A PENALTY METHOD FOR CORRELATION MATRIX PROBLEMS WITH PRESCRIBED CONSTRAINTS

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Summary

In many practical areas, people are interested in finding a nearest correlation matrix in the following sense:

$$\begin{array}{ll} \min & \frac{1}{2}\|H \circ (X - G)\|_F^2 \\ \text{s.t.} & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\ & X_{ij} = e_{ij}\,, \quad (i, j) \in \mathcal{B}_e\,, \\ & X_{ij} \geq l_{ij}\,, \quad (i, j) \in \mathcal{B}_l\,, \\ & X_{ij} \leq u_{ij}\,, \quad (i, j) \in \mathcal{B}_u\,, \\ & X \in \mathcal{S}_+^n\,. \end{array} \tag{1}$$

In model (1), the target matrix is positive semidefinite. Moreover, it is required to satisfy some prescribed constraints on its components. Thus the problem may become infeasible. To deal with this potential problem in model (1), we will borrow the essential idea of the exact penalty method via considering the penalized version by taking a trade-off between the prescribed constraints and the weighted least squares distance as follows:

$$
\begin{aligned}
\min \quad & F_\rho(X, r, v, w) \\
\text{s.t.} \quad & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\
& X_{ij} - e_{ij} = r_{ij}\,, \quad (i,j) \in \mathcal{B}_e\,, \\
& l_{ij} - X_{ij} = v_{ij}\,, \quad (i,j) \in \mathcal{B}_l\,, \\
& X_{ij} - u_{ij} = w_{ij}\,, \quad (i,j) \in \mathcal{B}_u\,, \\
& X \in \mathcal{S}^n_+\,,
\end{aligned}
\tag{2}
$$

where

$$
\begin{aligned}
F_\rho(X, r, v, w) := \frac{1}{2}\|H \circ (X - G)\|_F^2 + \rho\Big(& \sum_{(i,j)\in\mathcal{B}_e} |r_{ij}| + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij}, 0) \\
& + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij}, 0)\Big)
\end{aligned}
$$

for a given penalty parameter $\rho > 0$ that controls the weights allocated to the prescribed constraints in the objective function.

To solve problem (2), we apply the idea of the majorization method by solving a sequence of unconstrained inner problems iteratively. Actually, the inner problem is produced by the Lagrangian dual approach. Since the objective function in the inner problem is not twice continuously differentiable, we investigate a semismooth Newton-CG method for solving the inner problem based on the strongly semismooth matrix valued function. The convergence analysis is also included to justify our algorithm. Finally, we implement our algorithm with numerical results reported for a number of examples.

Chapter 1

Introduction

The nearest correlation matrix (NCM) problem is an important optimization model with many applications in statistics, finance and risk management and etc. In 2002, Higham [11] considered the following correlation matrix problem:

$$\begin{aligned} \min \quad & \frac{1}{2}\|H \circ (X - G)\|_F^2 \\ \text{s.t.} \quad & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\ & X \in \mathcal{S}^n_+\,, \end{aligned} \tag{1.1}$$

where $\mathcal{S}^n$ is the real Euclidean space of $n \times n$ symmetric matrices; $\mathcal{S}^n_+$ is the cone of all positive semidefinite matrices in $\mathcal{S}^n$; $\|\cdot\|_F$ denotes the Frobenius norm induced by the trace inner product $\langle A, B\rangle = \text{Tr}(AB)$, for any $A, B \in \mathcal{S}^n$; "$\circ$" denotes the Hadamard product $A \circ B = [A_{ij}B_{ij}]^n_{i,j=1}$, for any $A, B \in \mathcal{S}^n$; The weighted matrix H is symmetric and $H_{ij} \geq 0$ for all $i, j = 1, \ldots, n$. If the size of problem (1.1) is small and medium, some public softwares based on the Interior-Point-Methods such as SeDuMi [36] and SDPT3 [37] can be applied to solve (1.1) directly, see Higham [11] and Toh, Tütüncü and Todd [38]. But if the size of (1.1) becomes large, there exist some difficulties to use IPMs. Recently, Qi and Sun [27] proposed an augmented Lagrangian dual approach for solving (1.1), which was fast and robust. Furthermore, if there is some additional information, we can naturally extend (1.1) to the following optimization problem:

$$
\begin{array}{ll}
\min & \frac{1}{2}\|H \circ (X - G)\|_F^2 \\
\text{s.t.} & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\
& X_{ij} = e_{ij}\,, \quad (i,j) \in \mathcal{B}_e\,, \\
& X_{ij} \geq l_{ij}\,, \quad (i,j) \in \mathcal{B}_l\,, \\
& X_{ij} \leq u_{ij}\,, \quad (i,j) \in \mathcal{B}_u\,, \\
& X \in \mathcal{S}^n_+\,,
\end{array}
\tag{1.2}
$$

where $\mathcal{B}_e$, $\mathcal{B}_l$ and $\mathcal{B}_u$ are three index subsets of $\{\ (i,j) \mid 1 \leq i < j \leq n\ \}$. $\mathcal{B}_e$, $\mathcal{B}_l$ and $\mathcal{B}_u$ satisfy the following relationships: 1) $\mathcal{B}_e \cap \mathcal{B}_l = \emptyset$; 2) $\mathcal{B}_e \cap \mathcal{B}_u = \emptyset$; 3) for any index $(i,j) \in \mathcal{B}_l \cap \mathcal{B}_u$, $-1 \leq l_{ij} < u_{ij} \leq 1$; 4) for any index $(i,j) \in \mathcal{B}_e \cup \mathcal{B}_l \cup \mathcal{B}_u$, $-1 \leq e_{ij}, l_{ij}, u_{ij} \leq 1$. Denote by q_e, q_l and q_u the cardinalities of $\mathcal{B}_e$, $\mathcal{B}_l$ and $\mathcal{B}_u$ respectively. Let $m := q_e + q_l + q_u$. Note that the inexact smoothing Newton method can be applied to solve problem (1.2), see Gao and Sun [9].

However, in practice, people should notice the following key issues: i) the target matrix in (1.2) is positive semidefinite; ii) the target matrix in (1.2) is asked to satisfy some prescribed constraints on its components. Thus, the problem may become infeasible. To solve problem (1.2), we apply the essential idea of the exact penalty method. Now we consider the penalized problem by taking a trade-off between the prescribed constraints and the weighted least squares distance as follows:

$$
\begin{array}{ll}
\min & F_\rho(X, r, v, w) \\
\text{s.t.} & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\
& X_{ij} - e_{ij} = r_{ij}\,, \quad (i,j) \in \mathcal{B}_e\,, \\
& l_{ij} - X_{ij} = v_{ij}\,, \quad (i,j) \in \mathcal{B}_l\,, \\
& X_{ij} - u_{ij} = w_{ij}\,, \quad (i,j) \in \mathcal{B}_u\,, \\
& X \in \mathcal{S}^n_+\,,
\end{array}
\tag{1.3}
$$

where

$$F_\rho(X,r,v,w) := \frac{1}{2}\|H\circ(X-G)\|_F^2 + \rho\Big(\sum_{(i,j)\in\mathcal{B}_e}|r_{ij}| + \sum_{(i,j)\in\mathcal{B}_l}\max(v_{ij},0) + \sum_{(i,j)\in\mathcal{B}_u}\max(w_{ij},0)\Big)$$

and $\rho > 0$ is a given penalty parameter that controls the allocated weight to the prescribed constraints in the objective function.

For simplicity, we define four linear operators $\mathcal{A}_1 : \mathcal{S}^n \to \Re^n$, $\mathcal{A}_2 : \mathcal{S}^n \to \Re^{q_e}$, $\mathcal{A}_3 : \mathcal{S}^n \to \Re^{q_l}$ and $\mathcal{A}_4 : \mathcal{S}^n \to \Re^{q_u}$ to characterize the constraints in (1.3), respectively, by

$$\mathcal{A}_1(X) := \mathrm{diag}(X)\,,$$
$$(\mathcal{A}_2(X))_{ij} := X_{ij}\,, \quad \text{for } (i,j)\in\mathcal{B}_e\,,$$
$$(\mathcal{A}_3(X))_{ij} := X_{ij}\,, \quad \text{for } (i,j)\in\mathcal{B}_l\,,$$
$$(\mathcal{A}_4(X))_{ij} := X_{ij}\,, \quad \text{for } (i,j)\in\mathcal{B}_u\,.$$

For each $X \in \mathcal{S}^n$, $\mathcal{A}_1(X)$ is defined to be the vector formed by the diagonal entries of X, $\mathcal{A}_2(X)$, $\mathcal{A}_3(X)$ and $\mathcal{A}_4(X)$ are three column vectors in $\Re^{q_e}$, $\Re^{q_l}$ and $\Re^{q_u}$ obtained by storing $X_{ij}, (i,j)\in\mathcal{B}_e$, $X_{ij}, (i,j)\in\mathcal{B}_l$ and $X_{ij}, (i,j)\in\mathcal{B}_u$ column by column respectively. Let $\mathcal{A} : \mathcal{S} \to \Re^m$ be defined by

$$\mathcal{A}(X) := \begin{bmatrix} \mathcal{A}_1(X) \\ \mathcal{A}_2(X) \\ -\mathcal{A}_3(X) \\ \mathcal{A}_4(X) \end{bmatrix}, \quad X \in \mathcal{S}^n\,. \tag{1.4}$$

We denote

$$b := \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}, \tag{1.5}$$

where $b_1 \in \Re^n$ is the vector of all ones, $b_2 := \{e_{ij}\}_{(i,j)\in\mathcal{B}_e}$, $b_3 := -\{l_{ij}\}_{(i,j)\in\mathcal{B}_l}$ and $b_4 := \{u_{ij}\}_{(i,j)\in\mathcal{B}_u}$. Finally we define that

$$y := \begin{bmatrix} \{0\}^n \\ r \\ v \\ w \end{bmatrix} \in \Re^m , \tag{1.6}$$

where r, v and w are three column vectors in $\Re^{q_e}$, $\Re^{q_l}$ and $\Re^{q_u}$ obtained by storing $r_{ij}, (i,j) \in \mathcal{B}_e$, $v_{ij}, (i,j) \in \mathcal{B}_l$ and $w_{ij}, (i,j) \in \mathcal{B}_u$ column by column respectively.

Given by the above preparations, (1.3) can be rewritten as:

$$\begin{array}{ll} \min & F_\rho(X, y) \\ \text{s.t.} & \mathcal{A}(X) = b + y \, , \\ & X \in \mathcal{S}^n_+ \, , \end{array} \tag{1.7}$$

where

$$F_\rho(X, y) := \frac{1}{2}\|H \circ (X - G)\|_F^2 + \rho\Big(\|r\|_1 + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij}, 0) + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij}, 0)\Big) \, .$$

In order to solve the above penalized problem (1.7), we will apply the essential idea of the majorization method by solving a sequence of unconstrained inner problems iteratively. We analyze the convergence properties to ensure the efficiency of our majorization method. In fact, the inner problem is generated by the well-known Lagrangian dual approach based on the metric projection and the Moreau-Yosida regularization. Since the objective function in the inner problem is not twice continuously differentiable, by taking advantage of the strongly semismooth, we propose a semismooth Newton-CG method to solve the inner problem. Moreover, we show that the positive definiteness of the generalized Hessian of the objective function is equivalent to the constraint nondegeneracy of the corresponding primal problem. At last, we test the algorithm with some numerical examples and report the corresponding numerical results. These numerical experiments show that our algorithm is efficient and robust.

We list some other useful notations in our thesis. The matrix $E \in \mathcal{S}^n$ denotes the matrix of all ones. $B_{\alpha\beta}$ denotes the submatrix of B indexed by α and β where α and β are the index subsets of $\{1, 2, \dots, n\}$. E^{ij} denotes the matrix whose (i, j)th entry is 1 and all other entries are zeros. For any vector x, $\mathrm{Diag}(x)$ denotes the diagonal matrix whose diagonal entries are the elements of x. $\mathcal{T}_K(x)$ denotes the tangent cone of K at x. $\mathrm{lin}\big(\mathcal{T}_K(x)\big)$ denotes the lineality space of $\mathcal{T}_K(x)$. $\mathcal{N}_K(x)$ denotes the normal cone of K at x. $\delta_K(\cdot)$ denotes the indicator function with respect to set K. $\mathrm{dist}(x, S)$ denotes the distance between a point x and a set S.

1.1 Outline of the thesis

The remaining parts of this thesis are organized as follows. In Chapter 2, we present some preliminaries to facilitate the later discussions. In Chapter 3, we introduce the majorization method to deal with (1.7) and analyze its convergence properties. Chapter 4 concentrates on the semismooth Newton-CG method for solving the inner problems and the convergence analysis. In Chapter 5, we discuss some implementation issues and report our numerical results. The last Chapter is about some conclusions.

Chapter 2

Preliminaries

In this chapter, we introduce some preliminaries which are very useful in our later discussions. The related references are listed in the bibliography.

2.1 Generalized Jacobian and semismoothness

Let $F : \mathcal{O} \subseteq \Re^n \to \Re^m$ be a locally Lipschitz continuous function on an open set $\mathcal{O}$. By Rademacher's theorem [32, Section 9.J], F is almost everywhere F(réchet)-differentiable in $\mathcal{O}$. Denote by $\mathcal{D}_F$ the set of points in $\mathcal{O}$ where F is F-differentiable. Let $F'(x) : \Re^n \to \Re^m$ be the derivative of F at $x \in \mathcal{O}$ and $F'(x)^* : \Re^m \to \Re^n$ be the adjoint of $F'(x)$. Then, the B-subdifferential of F at $x \in \mathcal{O}$, denoted by $\partial_B F(x)$, is

$$\partial_B F(x) = \{ \lim_{x^k \to x} F'(x^k) \, , x^k \in \mathcal{D}_F \} \, . \tag{2.1}$$

Clarke's generalized Jacobian of F at x is defined as the convex hull of $\partial_B F(x)$, i.e.,

$$\partial F(x) = \text{conv}\{\partial_B F(x)\} \, . \tag{2.2}$$

We proceed to summarize some useful properties of ∂F, see [7, Proposition 2.6.2].

Proposition 2.1.1.

a) ∂F is a nonempty convex compact subset of $\Re^{m\times n}$.

b) ∂F is closed at x; that is, if $x_i \to x$, $Z_i \in \partial F(x_i)$, $Z_i \to Z$, then $Z \in \partial F(x)$.

To facilitate the latter discussions, we borrow the concept of semismoothness, which is first introduced in [22] and later extended to vector-valued function, see [28, 29].

Definition 2.1.1. F is said to be semismooth at x if

a) F is directionally differentiable at x; and

b) for any $h \in \Re^n$ and $V \in \partial F(x+h)$ with $h \to 0$,

$$F(x+h) - F(x) - Vh = o(\|h\|).$$

Furthermore, F is said to be strongly semismooth at x if F is semismooth at x and for any $h \in \Re^n$ and $V \in \partial F(x+h)$ with $h \to 0$,

$$F(x+h) - F(x) - Vh = O(\|h\|^2).$$

More details of the strongly semismooth can be found in [6, 34].

2.2 The matrix valued function and Löwner's operator

Let $X \in \mathcal{S}^n$ admit the following spectral decomposition:

$$X = P\text{diag}(\lambda(X))P^T, \tag{2.3}$$

$\lambda_1(X) \geq \cdots \geq \lambda_n(X)$ are the eigenvalues of X being arranged in the the non-increasing order and $P \in \mathcal{O}^n$ is the corresponding orthogonal matrix of orthonormal eigenvectors of X.

Let $\phi : \mathcal{R} \to \mathcal{R}$ be a scalar function, then the corresponding Löwner's operator matrix valued function at X is defined by [20]

$$\phi_{\mathcal{S}^n}(X) := \sum_{j=1}^{n} \phi(\lambda_j)(X) P_j P_j^T = P\mathrm{diag}\big(\,\phi(\lambda_1(X))\,,\,\phi(\lambda_2(X))\,,\cdots,\,\phi(\lambda_n(X))\,\big)P^T.$$

For Löwner's operator, the following theorem is often very useful. More details can be found in [6, 14].

Theorem 2.2.1. If X has spectral decomposition as in (2.3), the function $\phi_{\mathcal{S}^n}$ is (continuously) differentiable at X if and only if ϕ is (continuously) differentiable at $\lambda_j(X)(j = 1, \cdots, n)$. In this case, the F(réchet) derivative of $\phi_{\mathcal{S}^n}$ at X, for any $H \in \mathcal{S}^n$ is given by

$$\phi'_{\mathcal{S}^n}(X)[H] = P(\phi^{[1]}(\Lambda) \circ (P^T H P))P^T,$$

where $\phi^{[1]}(\Lambda)$ is the first-order divided difference matrix whose entries $\phi^{[1]}(\lambda_i, \lambda_j)$ $(i, j = 1, 2, \cdots, n)$ are defined as

$$\phi^{[1]}(\lambda_i, \lambda_j) = \begin{cases} \frac{\phi(\lambda_i) - \phi(\lambda_j)}{\lambda_i - \lambda_j} & \text{if } \lambda_i \neq \lambda_j, \\ \phi'(\lambda_i) & \text{if } \lambda_i = \lambda_j. \end{cases}$$

2.3 The metric projection operator $\Pi_{\mathcal{S}^n_+}(\cdot)$

For $X \in \mathcal{S}^n$, let $\Pi_{\mathcal{S}^n_+}(X)$ be the metric projection of X onto S^n_+. Suppose that X has the spectral decomposition as in (2.3). Then

$$\Pi_{\mathcal{S}^n_+}(X) = P\Lambda_+ P^T,$$

where Λ_+ is a diagonal matrix whose diagonal entries are the nonnegative parts of the respective diagonal entries of Λ, i.e.,

$$\Lambda_+ := \mathrm{Diag}\big(\max(\,\lambda_1(X)\,,0\,)\,,\cdots,\max(\,\lambda_n(X)\,,0\,)\big).$$

In [34], Sun and Sun demonstrate that $\Pi_{\mathcal{S}^n_+}(\cdot)$ is strongly semismooth everywhere in $\mathcal{S}^n$.

Define three index sets of positive, zero and negative eigenvalues of $\lambda(X)$, respectively, as

$$\alpha^* := \{\, i \,:\, \lambda_i(X) > 0\,\}, \quad \beta^* := \{\, i \,:\, \lambda_i(X) = 0\,\}, \quad \gamma^* := \{\, i \,:\, \lambda_i(X) < 0\,\}.$$

Recall the contents in section 2, let $U_X : \mathcal{S}^n \longrightarrow \mathcal{S}^n$ be defined by

$$U_X H = P(W_X \circ (P^T H P))P^T, \quad \text{for } H \in S^n, \tag{2.4}$$

where

$$W_X := \begin{bmatrix} E_{\alpha^*\alpha^*} & E_{\alpha^*\beta^*} & (v_{ij})_{\substack{i\in\alpha^*\\ j\in\gamma^*}} \\ E^T_{\alpha^*\beta^*} & 0 & 0 \\ (v_{ji})_{\substack{i\in\alpha^*\\ j\in\gamma^*}} & 0 & 0 \end{bmatrix}, \quad v_{ij} = \frac{\lambda_i(X)}{\lambda_i(X) - \lambda_j(X)}, \; i \in \alpha^*, \; j \in \gamma^*. \tag{2.5}$$

In [24], Pang, Sun and Sun show that $U_X \in \partial_B \Pi_{\mathcal{S}^n_+}(X)$.

In general, let K be a closed convex set in a finite dimensional real Hilbert space. It is famous that the metric projector $\Pi_K(\cdot)$ is globally Lipschitz continuous with modulus 1 and $\|z - \Pi_K(z)\|^2$ is continuously differentiable. More details can be found in [40].

Moreover, we introduce the concept of Jacobian amicability, see [2].

Definition 2.3.1. The metric projector $\Pi_K(\cdot)$ is Jacobian amicable at $x \in \mathcal{X}$ if for any $V \in \partial\Pi_K(x)$ and $d \in \mathcal{X}$ such that $Vd = 0$, it holds that

$$d \in \big(\mathrm{lin}(\mathcal{T}_K(\Pi_K(x)))\big)^\perp, \tag{2.6}$$

where $\big(\mathrm{lin}(\mathcal{T}_K(\Pi_K(x)))\big)^\perp$ is defined by

$$\big(\mathrm{lin}(\mathcal{T}_K(\Pi_K(x)))\big)^\perp := \{\, d \in \mathcal{X} \,:\, \langle d \,,\, h\rangle = 0 \,,\; \forall\, h \in \mathrm{lin}(\mathcal{T}_K(\Pi_K(x)))\,\}\,. \tag{2.7}$$

$\Pi_K(\cdot)$ is said to be Jacobian amicable if it is Jacobian amicable at every point in $\mathcal{X}$.

The following proposition is useful in the later discussions, see [2, Proposition 2.10].

Proposition 2.3.1. The projection operator $\Pi_{\mathcal{S}^n_+}(\cdot)$ is Jacobian amicable everywhere in $\mathcal{S}^n$.

2.4 The Moreau-Yosida regularization

Let $f : \mathcal{E} \to (-\infty, +\infty]$ be a closed proper convex function. The Moreau-Yosida regularization of f at $x \in \mathcal{E}$ is defined by

$$\psi_f(x) := \min_{y\in\mathcal{E}} f(y) + \frac{1}{2}\|y - x\|^2. \tag{2.8}$$

The unique optimal solution of (2.8), denoted by $P_f(x)$, is called the proximal point of x associated with f. The following results are useful in our thesis. They mainly comes from [30, 33].

Proposition 2.4.1. Let $f : \mathcal{E} \to (-\infty, +\infty]$ be a closed proper convex function, ψ_f be the Moreau-Yosida regularization of f and P_f be the associated proximal point mapping. Then, ψ_f is continuously differentiable. Furthermore, it holds that

$$\nabla\psi_f(x) = Q_f(x) = x - P_f(x), \quad x \in \mathcal{E}. \tag{2.9}$$

Proposition 2.4.2. Let f be a closed proper convex function on $\mathcal{E}$. For any $x \in \mathcal{E}$, $\partial P_f(x)$ has the following two properties:

(i) Any $V \in \partial P_f(x)$ is self-adjoint.

(ii) $\langle Vd,\, d\rangle \geq \|Vd\|^2$ for any $V \in \partial P_f(x)$ and $d \in \mathcal{E}$.

Theorem 2.4.1 (Moreau decomposition)**.** Let $f : \mathcal{E} \to (-\infty, +\infty]$ be a closed proper convex function and f^* be its conjugate. Then any $x \in \mathcal{E}$ has the decomposition

$$x = P_f(x) + P_{f^*}(x). \tag{2.10}$$

As an important application in our thesis, we introduce the following example. Let $f(x) = \|x\|_\#$ be any norm function defined on $\mathcal{E}$ and $\|\cdot\|_*$ be the dual norm of $\|\cdot\|_\#$, i.e., for any $x \in \mathcal{E}$, $\|x\|_* = \sup_{y\in\mathcal{E}}\{\langle x, y\rangle : \|y\|_\# \leq 1\}$. Since f is a positively homogeneous convex function, the conjugate function f^* must be the indicator function of $\partial f(0)$. Direct calculation shows that

$$\partial f(0) = B_*^1 := \{x \in \mathcal{E} : \|x\|_* \leq 1\}.$$

Therefore, $P_{f^*}(x) = \Pi_{B_*^1}(x)$ for any $x \in \mathcal{E}$. According to the Moreau decomposition, it holds that $P_f(x) = x - P_{f^*}(x) = x - \Pi_{B_*^1}(x)$.

Chapter 3

A Majorization Method

3.1 Introduction

This section is devoted to giving an general introduction to the majorization method.

Let $F : \Re^n \to \Re$ be a continuous function and $K \subset \Re^n$ be a closed convex set. We consider the following optimization problem:

$$\begin{array}{ll} \min & F(x) \\ \text{s.t.} & x \in K\,. \end{array} \tag{3.1}$$

The function $\hat{F}^k(x)$ is said to be the majorization function of $F(x)$ at x^k for $k \geq 0$ if it satisfies

$$\hat{F}^k(x^k) = F(x^k) \text{ and } \hat{F}^k(x) \geq F(x^k)\,, \quad \forall\, x \in K\,. \tag{3.2}$$

The procedures of a majorization method for solving (3.1) are mainly summarized as follows. Firstly, we properly choose an initial guess $x^0 \in K$. Secondly, for any $k \geq 0$, we minimize the function $\hat{F}^k(x)$ over the set K to obtain the optimal solution x^{k+1} iteratively.

In order to apply the majorization method efficiently, we must consider the following issues carefully: i) to obtain a fast convergence, the majorization functions may approximate the original function; ii) to solve the generated optimization problems more easily, the majorization functions may be simpler than the original function. These two issues often contradict with each other. We should deal with this dilemma according to the specific problem. Interested readers can refer to [12, 13, 16, 17, 19, 23] for more details about the majorization method.

3.2 The majorization method for the penalized problem

Write $\mathcal{F} = \{X \in \mathcal{S}^n \mid X \succeq 0, X_{ii} = 1, 1 \leq i \leq n\}$ and $\delta_{\mathcal{F}}(\cdot)$ as its indicator function. It is clear to see that the problem (1.2) is equivalent to

$$\begin{array}{ll} \min & \frac{1}{2}\|H \circ (X - G)\|^2 + \delta_{\mathcal{F}}(X) \\ s.t. & X_{ij} = e_{ij}\,, \quad (i,j) \in \mathcal{B}_e\,, \\ & X_{ij} \geq l_{ij}\,, \quad (i,j) \in \mathcal{B}_l\,, \\ & X_{ij} \leq u_{ij}\,, \quad (i,j) \in \mathcal{B}_u\,. \end{array} \tag{3.3}$$

As we have already mentioned in the introduction, the intersection of $\mathcal{F}$ and the feasible set defined by the constraints of (3.3) may be empty, which motivates us to apply the essential idea of the nonsmooth penalty method to (3.3). This yields the penalized problem

$$\begin{aligned} \min \frac{1}{2}\|H \circ (X - G)\|_F^2 + \rho\Big(\sum_{(i,j)\in\mathcal{B}_e} |X_{ij} - e_{ij}| + \sum_{(i,j)\in\mathcal{B}_l} \max(l_{ij} - X_{ij}, 0) \\ + \sum_{(i,j)\in\mathcal{B}_u} \max(X_{ij} - u_{ij}, 0)\Big) + \delta_{\mathcal{F}}(X), \end{aligned}$$

or equivalent problem (1.7), where ρ is some positive penalty parameter. It may be also noteworthy that our penalized method is exact since, by [8, Theorem 4.2], if the original problem is feasible and the corresponding Lagrangian multipliers associated with (3.3) exist, then the penalized problem (1.7) has the same solution set as the problem (1.2) for all ρ greater than some positive threshold which is related to the Lagrangian multipliers. See [3, 4] for more details of the exact penalization.

Now we focus on the penalized problem (1.7). Note that in (1.7), the objective function is

$$\frac{1}{2}\|H \circ (X-G)\|_F^2 + \rho\Big(\|r\|_1 + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij},0) + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij},0)\Big).$$

In order to design an efficient majorization method for solving (1.7), we first need to find the proper majorization functions of

$$\frac{1}{2}\|H \circ (X-G)\|_F^2$$

and

$$\rho\Big(\|r\|_1 + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij},0) + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij},0)\Big),$$

respectively. For simplicity, let y be defined in (1.6), let $g_1(X,y)$ be defined by

$$g_1(X,y) := \frac{1}{2}\|H \circ (X-G)\|_F^2, \tag{3.4}$$

let $g_2(X,y)$ be defined by

$$g_2(X,y) := \|r\|_1 + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij},0) + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij},0) \tag{3.5}$$

and let K denote the feasible set of problem (1.7), i.e.,

$$K = \{\, (X,y) : \; X \in \mathcal{S}^n_+ ,\; \mathcal{A}(X) = b + y \,\}.$$

For any (X,y) and (X^k,y^k) in K, let $\hat{g}_1(X,y;X^k,y^k)$ be defined by

$$\begin{aligned}\hat{g}_1(X,y;X^k,y^k) := & \frac{1}{2}\|H \circ (X^k-G)\|_F^2 + \langle H \circ H \circ (X^k-G)\,,\, X-X^k\rangle \\ & + \frac{\alpha}{2}\|X-X^k\|_F^2\end{aligned} \tag{3.6}$$

and let $\hat{g}_2(X, y; X^k, y^k)$ be defined by

$$\hat{g}_2(X, y; X^k, y^k) := \|r\|_1 + \frac{\beta}{2}\|r - r^k\|^2 + \sum_{(i,j)\in\mathcal{B}_l} (\max(v_{ij}, 0) + \frac{\beta}{2}|v_{ij} - v_{ij}^k|^2) + \sum_{(i,j)\in\mathcal{B}_u} (\max(w_{ij}, 0) + \frac{\beta}{2}|w_{ij} - w_{ij}^k|^2), \tag{3.7}$$

where α is larger than or equal to the Lipschitz constant of $\nabla_X g_1(X, y)$ and β is a fixed positive number. Obviously, $\hat{g}_2(X, y; X^k, y^k)$ is a majorization function of $g_2(X, y)$ due to the definition (3.2). Next, we prove that $\hat{g}_1(X, y; X^k, y^k)$ is also a majorization function of $g_1(X, y)$.

Proposition 3.2.1. For all (X^k, y^k) and (X, y) in K, $\hat{g}_1(X, y; X^k, y^k)$ is a majorization function of $g_1(X, y)$.

Proof. For all (X^k, y^k) and (X, y) in K, we have

$$\begin{aligned}
& |\, g_1(X, y) - g_1(X^k, y^k) - \langle \nabla_X g_1(X^k, y^k)\,,\, X - X^k\rangle \,| \\
= \;& |\int_0^1 \langle \nabla_X g_1(X^k + \theta(X - X^k), y^k) - \nabla_X g_1(X^k, y^k)\,,\, X - X^k\rangle d\theta| \\
\leq \;& \int_0^1 |\langle \nabla_X g_1(X^k + \theta(X - X^k), y^k) - \nabla_X g_1(X^k, y^k)\,,\, X - X^k\rangle| d\theta \\
\leq \;& \int_0^1 \|\nabla_X g_1(X^k + \theta(X - X^k), y^k) - \nabla_X g_1(X^k, y^k)\|_F \cdot \|X - X^k\|_F d\theta \\
\leq \;& \int_0^1 \theta L \|X - X^k\|_F^2 d\theta \\
= \;& \frac{L}{2}\|X - X^k\|_F^2,
\end{aligned}$$

where L is the Lipschitz constant of $\nabla_X g_1(\cdot)$. Since $\alpha \geq L$, it follows that

$$\begin{aligned}
& g_1(X, y) \\
\leq \;& g_1(X^k, y^k) + \langle \nabla_X g_1(X^k, y^k)\,,\, X - X^k\rangle + \frac{L}{2}\|X - X^k\|_F^2 \\
\leq \;& \frac{1}{2}\|H \circ (X^k - G)\|_F^2 + \langle H \circ H \circ (X^k - G)\,,\, X - X^k\rangle + \frac{\alpha}{2}\|X - X^k\|_F^2 \\
= \;& \hat{g}_1(X, y; X^k, y^k).
\end{aligned}$$

The proof is completed. □

Now, we can present the algorithm of the majorization method for solving the problem (1.7).

Algorithm 1 (Majorization Method) :

Step 0. Select a proper penalty parameter $\rho > 0$. Start to solve problem (1.7).

Step 1. Set $k := 0$. Choose an initial point $(X^0, y^0) \in K$ properly.

Step 2. By applying (3.6) and (3.7), respectively generate the majorization functions of $g_1(\cdot)$ and $g_2(\cdot)$ as

$$\hat{g}_1^k(\cdot) = \hat{g}_1(\cdot\,; X^k, y^k)$$

and

$$\hat{g}_2^k(\cdot) = \hat{g}_2(\cdot\,; X^k, y^k).$$

Due to (3.2), at (X^k, y^k), $F_\rho(\cdot)$ is majorized by

$$\hat{F}_\rho^k(\cdot) := \hat{F}_\rho(\cdot\,; X^k, y^k) = \hat{g}_1(\cdot\,; X^k, y^k) + \rho\hat{g}_2(\cdot\,; X^k, y^k) = \hat{g}_1^k(\cdot) + \rho\hat{g}_2^k(\cdot)\,.$$

Then solve the following optimization problem

$$\begin{array}{ll} \min & \hat{F}_\rho^k(X, y) \\ \text{s.t.} & (X, y) \in K \end{array} \tag{3.8}$$

to obtain the optimal solution (X^{k+1}, y^{k+1}).

Step 3. If $X^{k+1} = X^k$ and $y^{k+1} = y^k$, stop; otherwise, set $k := k + 1$ and go to Step 2.

3.3 Convergence analysis

In this section, we discuss the convergence analysis of the majorization method. We first prove the following lemma.

Lemma 3.3.1. Let $\{(X^k, y^k)\}$ be the sequence generated by Algorithm 1. Then the following two conclusions hold:

i) $\{F_\rho(X^k, y^k)\}$ is a nonincreasing sequence.

ii) The infinite sequence $\{F_\rho(X^k, y^k)\}$ satisfies

$$\frac{\alpha}{2}\|X^{k+1}-X^k\|_F^2+\frac{\rho\beta}{2}\|y^{k+1}-y^k\|^2 \leq F_\rho(X^k, y^k)-F_\rho(X^{k+1}, y^{k+1}),\ k = 0, 1, \cdots .$$

Proof. i) Firstly, by the definition of majorization function as in (3.2), it is obvious that

$$\hat{F}_\rho^k(X^k, y^k) = F_\rho(X^k, y^k)\,, \quad \forall\ k \geq 0\,.$$

Secondly, since (X^{k+1}, y^{k+1}) is an optimal solution to problem (3.8), then

$$\hat{F}_\rho^k(X^{k+1}, y^{k+1}) \leq \hat{F}_\rho^k(X^k, y^k), \quad \forall\ k \geq 0.$$

Thirdly, by applying Proposition 3.2.1, for any (X^k, y^k) and (X^{k+1}, y^{k+1}) in K, we obtain that

$$g_1(X^{k+1}, y^{k+1}) \leq \hat{g}_1(X^{k+1}, y^{k+1}; X^k, y^k) = \hat{g}_1^k(X^{k+1}, y^{k+1}). \tag{3.9}$$

In addition, by the definition of $g_2(\cdot)$ as in (3.5) and the definition of $\hat{g}_2(\cdot)$ as in (3.7), obviously,

$$g_2(X^{k+1}, y^{k+1}) \leq \hat{g}_2(X^{k+1}, y^{k+1}; X^k, y^k) = \hat{g}_2^k(X^{k+1}, y^{k+1}). \tag{3.10}$$

Furthermore, by combining (3.9) and (3.10), we establish that

$$F_\rho(X^{k+1}, y^{k+1}) \leq \hat{F}_\rho^k(X^{k+1}, y^{k+1}), \quad \forall\ k \geq 0.$$

Thus, we complete the proof by noting that

$$F_\rho(X^{k+1}, y^{k+1}) \leq \hat{F}_\rho^k(X^{k+1}, y^{k+1}) \leq \hat{F}_\rho^k(X^k, y^k) = F_\rho(X^k, y^k), \quad \forall\ k \geq 0.$$

ii) Since (X^{k+1}, y^{k+1}) is an optimal solution to problem (3.8), it holds that

$$0 \in \begin{bmatrix} \nabla_X g_1(X^k, y^k) + \alpha(X^{k+1} - X^k) \\ \rho\beta(y^{k+1} - y^k) \end{bmatrix} + \begin{bmatrix} 0 \\ \partial_y(\rho g_2(X^{k+1}, y^{k+1})) \end{bmatrix} + \mathcal{N}_K(X^{k+1}, y^{k+1}).$$

Then there exist

$$\tau^{k+1} \in \partial_y(\rho g_2(X^{k+1}, y^{k+1}))$$

and

$$\begin{bmatrix} \xi_1^{k+1} \\ \xi_2^{k+1} \end{bmatrix} \in \mathcal{N}_K(X^{k+1}, y^{k+1})$$

such that

$$\begin{bmatrix} \nabla_X g_1(X^k) + \alpha(X^{k+1} - X^k) \\ \rho\beta(y^{k+1} - y^k) \end{bmatrix} + \begin{bmatrix} 0 \\ \tau^{k+1} \end{bmatrix} + \begin{bmatrix} \xi_1^{k+1} \\ \xi_2^{k+1} \end{bmatrix} = 0. \tag{3.11}$$

Moreover, by recalling the properties of normal cone, we obtain

$$\langle \xi_1^{k+1}, X^k - X^{k+1} \rangle \leq 0 \tag{3.12}$$

and

$$\langle \xi_2^{k+1}, y^k - y^{k+1} \rangle \leq 0. \tag{3.13}$$

Therefore, by applying (3.11), (3.12) and (3.13), for each $k \geq 0$, it follows that

$$
\begin{aligned}
& F_\rho(X^k, y^k) - F_\rho(X^{k+1}, y^{k+1}) \\
= \;& g_1(X^k, y^k) + \rho g_2(X^k, y^k) - g_1(X^{k+1}, y^{k+1}) - \rho g_2(X^{k+1}, y^{k+1}) \\
\geq \;& g_1(X^k, y^k) + \rho g_2(X^k, y^k) - \big(g_1(X^k, y^k) + \langle \nabla_X g_1(X^k, y^k)\,,\, X^{k+1} - X^k\rangle \\
& + \frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2 + \rho g_2(X^{k+1}, y^{k+1}) + \frac{\rho\beta}{2}\|y^{k+1} - y^k\|^2\big) \\
= \;& -\langle \nabla_X g_1(X^k, y^k)\,,\, X^{k+1} - X^k\rangle - \frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2 + \rho g_2(X^k, y^k) \\
& - \rho g_2(X^{k+1}, y^{k+1}) - \frac{\rho\beta}{2}\|y^{k+1} - y^k\|^2 \\
\geq \;& -\langle \nabla_X g_1(X^k, y^k), X^{k+1} - X^k\rangle - \frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2 + \langle \tau^{k+1}\,,\, y^k - y^{k+1}\rangle \\
& + \langle \xi_1^{k+1}\,,\, X^k - X^{k+1}\rangle + \langle \xi_2^{k+1}\,,\, y^k - y^{k+1}\rangle - \frac{\rho\beta}{2}\|y^{k+1} - y^k\|^2 \\
= \;& \langle -\nabla_X g_1(X^k, y^k) - \xi_1^{k+1}\,,\, X^{k+1} - X^k\rangle - \frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2 \\
& + \langle -\tau^{k+1} - \xi_2^{k+1}\,,\, y^{k+1} - y^k\rangle - \frac{\rho\beta}{2}\|y^{k+1} - y^k\|^2 \\
= \;& \frac{\alpha}{2}\|X^{k+1} - X^k\|_F^2 + \frac{\rho\beta}{2}\|^{k+1} - y^k\|^2.
\end{aligned}
$$

The proof is complete. □

Now, we are ready to prove the convergence of the majorization method.

Theorem 3.3.1. Let $\{(X^k, y^k)\}$ be the sequence generated by the Algorithm 1. Then the following three conclusions hold:

i) The infinite sequence $\{(X^k, y^k)\}$ is bounded.

ii) Any accumulation point (X^*, y^*) of $\{(X^k, y^k)\}$ is a solution to the penalized problem (1.7).

iii) The sequence $\{F_\rho(X^k, y^k)\}$ converges to the optimal value of (1.7).

Proof. i) Obviously, the infinite sequence $\{X^k\}$ is bounded as the feasible set K is bounded. Furthermore, by applying i) in Lemma 3.3.1, the infinite sequence $\{y^k\}$

is bounded because the sequence $\{y^k\}$ satisfy

$$\|y^k\|_1 \leq F_\rho(X^0, y^0), \quad \text{for each } k \geq 0.$$

Thus, the infinite sequence $\{(X^k, y^k)\}$ is bounded.

ii) Assume that $\{(X^*, y^*)\}$ is an arbitrary accumulation point of $\{(X^k, y^k)\}$. Let $\{(X^{n_k}, y^{n_k})\}$ be a subsequence of $\{(X^k, y^k)\}$ such that $\{(X^{n_k}, y^{n_k})\}$ converges to (X^*, y^*). Since (X^{n_k+1}, y^{n_k+1}) is an optimal solution to the following problem

$$\begin{array}{ll} \min & \hat{F}_\rho^{n_k}(X, y) \\ \text{s.t.} & (X, y) \in K\,, \end{array}$$

we obtain that

$$\begin{aligned} 0 \in & \begin{bmatrix} \nabla_X g_1(X^{n_k}, y^{n_k}) + \alpha(X^{n_k+1} - X^{n_k}) \\ \rho\beta(y^{n_k+1} - y^{n_k}) \end{bmatrix} \\ & + \begin{bmatrix} 0 \\ \partial_y(\rho g_2(X^{n_k+1}, y^{n_k+1})) \end{bmatrix} + \mathcal{N}_K(X^{n_k+1}, y^{n_k+1})\,, \end{aligned}$$

which is equivalent to

$$\begin{aligned} - \begin{bmatrix} \nabla_X g_1(X^{n_k}, y^{n_k}) + \alpha(X^{n_k+1} - X^{n_k}) \\ \rho\beta(y^{n_k+1} - y^{n_k}) \end{bmatrix} \in & \begin{bmatrix} 0 \\ \partial_y(\rho g_2(X^{n_k+1}, y^{n_k+1})) \end{bmatrix} \\ & + \mathcal{N}_K(X^{n_k+1}, y^{n_k+1}). \end{aligned} \tag{3.14}$$

In addition, by the continuity of $g_1(\cdot)$, it follows that

$$\nabla_X g_1(X^{n_k}, y^{n_k}) \to \nabla_X g_1(X^*, y^*), \quad \text{as} \quad k \to \infty. \tag{3.15}$$

Furthermore, by ii) in Lemma 3.3.1, we have

$$\sum_{k=0}^{\infty} \frac{\alpha}{2}\|X^{n_k+1} - X^{n_k}\|_F^2 + \sum_{k=0}^{\infty} \frac{\rho\beta}{2}\|y^{n_k+1} - y^{n_k}\|^2 \leq F_\rho(X^0, y^0) - F_\rho(X^*, y^*),$$

which implies that

$$\alpha(X^{n_k+1} - X^{n_k}) \to 0, \quad \text{as} \quad k \to \infty \tag{3.16}$$

and

$$\rho\beta(y^{n_k+1} - y^{n_k}) \to 0, \quad \text{as} \quad k \to \infty. \tag{3.17}$$

Hence, by combining (3.14), (3.15), (3.16), (3.17) and (b) in Proposition 2.1.1 of Chapter 2, we know that

$$-\begin{bmatrix} \nabla_X g_1(X^*, y^*) \\ 0 \end{bmatrix} \in \begin{bmatrix} 0 \\ \partial_y(\rho g_2(X^*, y^*)) \end{bmatrix} + \mathcal{N}_K(X^*, y^*)\,,$$

which equivalently means $\{(X^*, y^*)\}$ is a solution to problem (1.7).

iii) Recall that $F_\rho(X^k, y^k)$ is a nonincreasing sequence by i) in Lemma 3.3.1 and it holds that

$$F_\rho(X^k, y^k) \geq 0, \quad \text{for all } k \geq 0,$$

thus this sequence admits a limit. By applying the previous conclusion, it follows that

$$\lim_{k\to\infty} F_\rho(X^k, y^k) = \lim_{k\to\infty} F_\rho(X^{n_k}, y^{n_k}) = F_\rho(X^*, y^*)\,.$$

This completes the proof. □

Chapter 4

A Semismooth Newton-CG Method

4.1 Introduction

In this section, we give an introduction to the nonsmooth Newton's method which is a generalization of the classical Newton's method.

Let $F : \Re^n \to \Re^n$ be a (locally) Lipschitz function. The nonsmooth Newton's method for solving $F(x) = 0$ is given by [29]

$$x^{k+1} = x^k - V_k^{-1} F(x^k), \quad V_k \in \partial F(x^k), \quad k = 0, 1, 2 \ldots, \tag{4.1}$$

where x^0 is an initial point.

A counterexample in [15] indicates that the above iterative method may not converge. However, Qi and Sun [29] show that the iterate sequence generated by (4.1) converges superlinearly if F is a semismooth function. In our thesis, it seems that the classical Newton's method is improper. Furthermore, there may not exist quadratic convergence. We mainly borrow the essential idea of Qi and Sun [25] to construct the inexact globalized semismooth Newton's method.

4.2 The semismooth Newton-CG method for the inner problem

In this section, we focus on the inner problem (3.8) generated in the kth step of Algorithm 1, which is equivalent to the optimization problem as follows:

$$\begin{array}{ll} \min & g(X,y) \\ \text{s.t.} & \mathcal{A}(X) = b + y\,, \\ & X \in \mathcal{S}^n_+\,, \end{array} \tag{4.2}$$

where

$$\begin{aligned} g(X,y) = {} & \frac{1}{2}\|H\circ(X^k - G)\|_F^2 + \langle H\circ H\circ(X^k - G)\,,\, X - X^k\rangle + \frac{\alpha}{2}\|X - X^k\|_F^2 \\ & + \rho\Big(\|r\|_1 + \frac{\beta}{2}\|r - r^k\|^2 + \sum_{(i,j)\in\mathcal{B}_l}(\max(v_{ij},0) + \frac{\beta}{2}|v_{ij} - v_{ij}^k|) \\ & + \sum_{(i,j)\in\mathcal{B}_u}(\max(w_{ij},0) + \frac{\beta}{2}|w_{ij} - w_{ij}^k|)\Big)\,, \end{aligned}$$

$\mathcal{A}$ is defined in (1.4), b is defined in (1.5) and y is defined in (1.6). The corresponding ordinary Lagrangian function $L(X,y,z) : \mathcal{S}^n_+ \times \Re^m \times \Re^m \to \Re$ is given by

$$L(X,y,z) := g(X,y) + \langle z, b - \mathcal{A}(X) + y\rangle\,. \tag{4.3}$$

To simplify the latter discussions, we give some notations and definitions in advance. For any $z_1 \in \Re^n$, $z_2 \in \Re^{q_e}$, $z_3 \in \Re^{q_l}$ and $z_4 \in \Re^{q_u}$, we denote $z := (z_1, z_2, z_3, z_4) \in \Re^n \times R^{q_e} \times \Re^{q_l} \times \Re^{q_u}$; Conversely, for any $z \in \Re^m$, we characterize $z := (z_1, z_2, z_3, z_4)$, where $z_1 \in \Re^n$, $z_2 \in \Re^{q_e}$, $z_3 \in \Re^{q_l}$ and $z_4 \in \Re^{q_u}$. The above relationships also extend to the sets

$$\{\,(h_1,h_2,h_3,h_4,h) :\; h_1 \in \Re^n,\; h_2 \in \Re^{q_e},\; h_3 \in \Re^{q_l},\; h_4 \in \Re^{q_u},\; h \in \Re^m\,\}$$

and

$$\{\,(d_1,d_2,d_3,d_4,d) :\; d_1 \in \Re^n,\; d_2 \in \Re^{q_e},\; d_3 \in \Re^{q_l},\; d_4 \in \Re^{q_u},\; d \in \Re^m\,\}.$$

Let $\mathcal{A}_1^*$, $\mathcal{A}_2^*$, $\mathcal{A}_3^*$ and $\mathcal{A}_4^*$ be the adjoints of $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$ and $\mathcal{A}_4$, respectively, defined by

$$\mathcal{A}_1^* x := \mathrm{Diag}(x), \quad \text{for} \;\; x \in \Re^n \,,$$

$$\mathcal{A}_2^* x := \frac{1}{2} \sum_{(i,j)\in\mathcal{B}_e} x_{ij}(E^{ij} + E^{ji}), \quad \text{for} \;\; x \in \Re^{q_e} \,,$$

$$\mathcal{A}_3^* x := \frac{1}{2} \sum_{(i,j)\in\mathcal{B}_l} x_{ij}(E^{ij} + E^{ji}), \quad \text{for} \;\; x \in \Re^{q_l}$$

and

$$\mathcal{A}_4^* x := \frac{1}{2} \sum_{(i,j)\in\mathcal{B}_u} x_{ij}(E^{ij} + E^{ji}), \quad \text{for} \;\; x \in \Re^{q_u} \,.$$

Obviously, in (4.2), $\mathcal{A} : \mathcal{S} \to \Re^m$ is surjective. The adjoint of $\mathcal{A}$ takes the following form:

$$\mathcal{A}^* z := \mathcal{A}_1^* z_1 + \mathcal{A}_2^* z_2 - \mathcal{A}_3^* z_3 + \mathcal{A}_4^* z_4, \quad z \in \Re^m.$$

Denote $f : \mathcal{S}^n \to \Re$ by

$$f(X) := \frac{1}{2}\|H \circ (X - G)\|_F^2, \quad X \in \mathcal{S}^n \,,$$

then,

$$\nabla f(X) = H \circ H \circ (X - G) \,.$$

Finally, we denote

$$D(z) := \frac{1}{\alpha}(\nabla f(X^k) - \mathcal{A}^* z)$$

and

$$C(z) := f(X^k) + \langle z, b - \mathcal{A}(X^k) + y^k \rangle - \frac{1}{2\rho\beta}\|z_2\|^2 - \frac{1}{2\rho\beta}\|z_3\|^2 - \frac{1}{2\rho\beta}\|z_4\|^2.$$

Given by the previous discussions, the Lagrangian dual problem of (4.2) is

$$\max_{z\in R^m} \inf_{\substack{X\in\mathcal{S}_+^n \\ y\in\Re^m}} L(X, y, z) \,. \tag{4.4}$$

Let $E : \Re^m \to \Re$ be defined by

$$E(z) := - \inf_{\substack{X \in \mathcal{S}^n_+ \\ y \in \Re^m}} L(X, y, z), \quad z \in \Re^m \,. \tag{4.5}$$

Then, (4.4) is equivalent to

$$\begin{aligned} \min \quad & E(z) \\ \text{s.t.} \quad & z \in \Re^m \,, \end{aligned} \tag{4.6}$$

where $E(z)$ can be written as

$$\begin{aligned} E(z) = - \inf_{\substack{X \in \mathcal{S}^n_+ \\ y \in \Re^m}} \Big[& \frac{\alpha}{2}(\|X - X^k + D(z)\|_F^2 - \|D(z)\|_F^2) + \rho(\|r\|_1 + \frac{\beta}{2}\|r - r^k + \frac{1}{\rho\beta}z_2\|^2) \\ & + \rho(\sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij}, 0) + \frac{\beta}{2}\|v - v^k + \frac{1}{\rho\beta}z_3\|^2) + \rho(\sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij}, 0) \\ & + \frac{\beta}{2}\|w - w^k + \frac{1}{\rho\beta}z_4\|^2) + C(z) \Big]. \end{aligned}$$

Recall the metric projection introduced in Section 2.3 of Chapter 2, we know that

$$X' = \Pi_{\mathcal{S}^n_+}(X^k - D(z)) \tag{4.7}$$

is the optimal solution to the optimization problem

$$\begin{aligned} \min \quad & \frac{\alpha}{2}(\|X - X^k + D(z)\|_F^2 - \|D(z)\|_F^2) \\ \text{s.t.} \quad & X \in \mathcal{S}^n_+ \,. \end{aligned}$$

Therefore, $E(z)$ can be equivalently written as

$$\begin{aligned} E(z) = & -\frac{\alpha}{2}(\|X^k - D(z) - \Pi_{\mathcal{S}^n_+}(X^k - D(z))\|_F^2 - \|D(z)\|_F^2) - \inf_{r\in\Re^{q_e}} \rho\beta(\frac{1}{\beta}\|r\|_1 \\ & + \frac{1}{2}\|r - (r^k - \frac{1}{\rho\beta}z_2)\|^2) - \inf_{v\in\Re^{q_l}} \rho\beta(\frac{1}{\beta}\sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij}, 0) \\ & + \frac{1}{2}\|v - (v^k - \frac{1}{\rho\beta}z_3)\|^2) - \inf_{w\in\Re^{q_u}} \rho\beta(\frac{1}{\beta}\sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij}, 0) \\ & + \frac{1}{2}\|w - (w^k - \frac{1}{\rho\beta}z_4)\|^2) - C(z). \end{aligned}$$

By applying Position 2.4.1 in Chapter 2, we respectively obtain

$$\nabla_{z_2}(\inf_{r\in\Re^{q_e}} \frac{1}{\beta}\|r\|_1 + \frac{1}{2}\|r - r^k + \frac{1}{\rho\beta}z_2\|^2) = -\frac{1}{\rho\beta}\Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(r^k - \frac{1}{\rho\beta}z_2)\,, \tag{4.8}$$

$$\begin{aligned} &\nabla_{(z_3)_{ij}}(\inf_{v_{ij}} \frac{1}{\beta}\max(v_{ij},0) + \frac{1}{2}\|v_{ij} - (v^k)_{ij} + \frac{1}{\rho\beta}(z_3)_{ij}\|^2) \\ = &\ -\frac{1}{\rho\beta}\Pi_{[0,\frac{1}{\beta}]}((v^k)_{ij} - \frac{1}{\rho\beta}(z_3)_{ij}), \quad (i,j)\in\mathcal{B}_l \end{aligned} \tag{4.9}$$

and

$$\begin{aligned} &\nabla_{(z_4)_{ij}}(\inf_{w_{ij}} \frac{1}{\beta}\max(w_{ij},0) + \frac{1}{2}\|w_{ij} - (w^k)_{ij} + \frac{1}{\rho\beta}(z_4)_{ij}\|^2) \\ = &\ -\frac{1}{\rho\beta}\Pi_{[0,\frac{1}{\beta}]}((w^k)_{ij} - \frac{1}{\rho\beta}(z_4)_{ij}), \quad (i,j)\in\mathcal{B}_u\,. \end{aligned} \tag{4.10}$$

Thus the gradient of E at z takes the following form:

$$\nabla_z E(z) = \begin{pmatrix} \mathcal{A}_1\Pi_{\mathcal{S}^n_+}(X^k - D(z)) \\ \mathcal{A}_2\Pi_{\mathcal{S}^n_+}(X^k - D(z)) + \Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(r^k - \frac{1}{\rho\beta}z_2) - r^k + \frac{1}{\rho\beta}z_2 \\ -\mathcal{A}_3\Pi_{\mathcal{S}^n_+}(X^k - D(z)) + \Pi_{[0,\frac{1}{\beta}]}(v^k - \frac{1}{\rho\beta}z_3) - v^k + \frac{1}{\rho\beta}z_3 \\ \mathcal{A}_4\Pi_{\mathcal{S}^n_+}(X^k - D(z)) + \Pi_{[0,\frac{1}{\beta}]}(w^k - \frac{1}{\rho\beta}z_4) - w^k + \frac{1}{\rho\beta}z_4 \end{pmatrix} - b\,. \tag{4.11}$$

For problem (4.2), the generalized Slater condition holds if

$$\begin{cases} \mathcal{A}:\mathcal{S}^n \to \Re^m \ \text{ is onto}\,, \\ \exists\ \overline{X}\in \operatorname{int}(\mathcal{S}^n_+),\ \bar{y}\in\Re^m \ \text{ such that }\ \mathcal{A}(\overline{X}) = b + \bar{y}\,, \end{cases} \tag{4.12}$$

where "int" denotes the topological interior of a given set. Under the generalized Slater condition, we know that the famous Lagrangian dual approach described in [31] holds. Hence, we can first solve the problem (4.6) to obtain a solution $z^*\in\Re^m$. Next, by applying the example introduced in Section 2.4 of Chapter 2, we know that the optimal solution to the following problem

$$\inf_{r\in\Re^{q_e}}(\frac{1}{\beta}\|r\|_1 + \frac{1}{2}\|r - r^k + \frac{1}{\rho\beta}z_2\|^2)$$

is

$$r' = P_{\frac{1}{\beta}\|\cdot\|_1}(r^k - \frac{1}{\rho\beta}z_2) = r^k - \frac{1}{\rho\beta}z_2 - \Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(r^k - \frac{1}{\rho\beta}z_2)\,. \tag{4.13}$$

Similarly, the optimal solution to the following problem

$$\inf_{v\in\Re^{q_l}}(\frac{1}{\beta}\sum_{(i,j)\in\mathcal{B}_l}\max(v_{ij},0) + \frac{1}{2}\|v - v^k + \frac{1}{\rho\beta}z_3\|^2)$$

is

$$\begin{aligned}(v')_{ij} &= P_{\frac{1}{\beta}\max(\cdot,0)}((v^k)_{ij} - \frac{1}{\rho\beta}(z_3)_{ij})\\ &= (v^k)_{ij} - \frac{1}{\rho\beta}(z_3)_{ij} - \Pi_{[0,\frac{1}{\beta}]}((v^k)_{ij} - \frac{1}{\rho\beta}(z_3)_{ij})\,, \quad (i,j)\in\mathcal{B}_l\end{aligned} \tag{4.14}$$

and the optimal solution to the following problem

$$\inf_{w\in\Re^{q_u}}(\frac{1}{\beta}\sum_{(i,j)\in\mathcal{B}_u}\max(w_{ij},0) + \frac{1}{2}\|w - w^k + \frac{1}{\rho\beta}z_4\|^2)$$

is

$$\begin{aligned}(w')_{ij} &= P_{\frac{1}{\beta}\max(\cdot,0)}((w^k)_{ij} - \frac{1}{\rho\beta}(z_4)_{ij})\\ &= (w^k)_{ij} - \frac{1}{\rho\beta}(z_4)_{ij} - \Pi_{[0,\frac{1}{\beta}]}((w^k)_{ij} - \frac{1}{\rho\beta}(z_4)_{ij})\,, \quad (i,j)\in\mathcal{B}_u\,.\end{aligned} \tag{4.15}$$

Finally, by applying (4.7), (4.13), (4.14) and (4.15), the solution (X^*, y^*) of (4.2) takes the following relationships as

$$X^* = \Pi_{\mathcal{S}^n_+}[X^k - \frac{1}{\alpha}(\nabla f(X^k) - \mathcal{A}^*z^*)]$$

and

$$y^* = \begin{bmatrix} 0 \\ r^* \\ v^* \\ w^* \end{bmatrix},$$

where

$$u^* = P_{\frac{1}{\beta}\|\cdot\|_1}(r^k - \frac{1}{\rho\beta}z_2^*) = r^k - \frac{1}{\rho\beta}z_2^* - \Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(r^k - \frac{1}{\rho\beta}z_2^*)\,,$$

$$v^* = P_{\frac{1}{\beta}\max(\cdot,0)}(v^k - \frac{1}{\rho\beta}z_3^*) = v^k - \frac{1}{\rho\beta}z_3^* - \Pi_{[0,\frac{1}{\beta}]}(v^k - \frac{1}{\rho\beta}z_3^*)$$

and

$$w^* = P_{\frac{1}{\beta}\max(\cdot,0)}(w^k - \frac{1}{\rho\beta}z_4^*) = w^k - \frac{1}{\rho\beta}z_4^* - \Pi_{[0,\frac{1}{\beta}]}(w^k - \frac{1}{\rho\beta}z_4^*)\,.$$

Note that the metric projector $\Pi_{\mathcal{S}_+^n}(\cdot)$, $\Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(\cdot)$ and $\Pi_{[0,\frac{1}{\beta}]}(\cdot)$ fails to be continuously differentiable. By observing (4.11), E can not be twice continuously differentiable. Fortunately, $\Pi_{\mathcal{S}_+^n}(\cdot)$, $\Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(\cdot)$ and $\Pi_{[0,\frac{1}{\beta}]}(\cdot)$ are strongly semismooth. In this situation, we borrow the idea of Qi and Sun [25] to construct a quadratically converging Newton's method to solve the problem (4.6).

Denote

$$F(z) := \nabla_z E(z), \quad z \in \Re^m$$

Note that $\Pi_K(\cdot)$ is globally Lipschitz continuous with modulus 1 when K is a closed convex set. Thus, F is Lipschitz continuous on $\Re^m$. From the contents in Section 2.1 of Chapter 2, we know that generalized Hessian of E at $z \in \Re^m$ is defined as

$$\partial^2 E(z) := \partial F(z) = \mathrm{conv}\{\partial_B F(z)\}.$$

For any $z \in \Re^m$, we define

$$\hat{\partial}^2 E(z) := \frac{1}{\alpha}\mathcal{A}\partial\Pi_{\mathcal{S}_+^n}(X^k - D(z))\mathcal{A}^*$$
$$+\frac{1}{\rho\beta}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & I_2 - \partial\Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(\hat{r}) & 0 & 0 \\ 0 & 0 & I_3 - \partial\Pi_{[0,\frac{1}{\beta}]}(\hat{v}) & 0 \\ 0 & 0 & 0 & I_4 - \partial\Pi_{[0,\frac{1}{\beta}]}(\hat{w}) \end{bmatrix},$$

where I_2 is an identity operator in $\Re^{q_e}$, I_3 is an identity operator in $\Re^{q_l}$, I_4 is an identity operator in $\Re^{q_u}$, $\hat{r} = r^k - \frac{1}{\rho\beta}z_2$, $\hat{v} = v^k - \frac{1}{\rho\beta}z_3$, $\hat{w} = w^k - \frac{1}{\rho\beta}z_4$ and

$\mathcal{A}\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}^*$ takes the form of

$\mathcal{A}\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}^* :=$

$$\begin{bmatrix} \mathcal{A}_1\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_1^* & \mathcal{A}_1\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_2^* & \mathcal{A}_1\partial\Pi_{\mathcal{S}^n_+}(\cdot)(-\mathcal{A}_3^*) & \mathcal{A}_1\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_4^* \\ \mathcal{A}_2\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_1^* & \mathcal{A}_2\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_2^* & \mathcal{A}_2\partial\Pi_{\mathcal{S}^n_+}(\cdot)(-\mathcal{A}_3^*) & \mathcal{A}_2\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_4^* \\ (-\mathcal{A}_3)\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_1^* & (-\mathcal{A}_3)\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_2^* & \mathcal{A}_3\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_3^* & (-\mathcal{A}_3)\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_4^* \\ \mathcal{A}_4\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_1^* & \mathcal{A}_4\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_2^* & \mathcal{A}_4\partial\Pi_{\mathcal{S}^n_+}(\cdot)(-\mathcal{A}_3^*) & \mathcal{A}_4\partial\Pi_{\mathcal{S}^n_+}(\cdot)\mathcal{A}_4^* \end{bmatrix}.$$

By [page75] in Clarke [7], for any $h \in \Re^m$, we have

$$\partial^2 E(z)h \subseteq \hat{\partial}^2 E(z)h.$$

Now, we can borrow the Algorithm 5.1 in [25] or Algorithm 3.1 in [26] to solve the problem (4.6).

Algorithm 2 (Semismooth Newton-CG Method) :

Step 0. Set the parameters as $\eta \in (0,1)$, $\mu \in (0,1)$, $\sigma \in (0,1/2)$. Choose an initial point $z^0 \in \Re^m$. Set $k := 0$.

Step 1. Compute an element $V_k \in \hat{\partial}^2 E(z^k)$. Then apply the CG (Hestenes and Stiefel [10]) or PCG to obtain a solution d^k for the following equation

$$\nabla E(z^k) + V_k d = 0 \tag{4.16}$$

satisfying

$$\|\nabla E(z^k) + V_k d^k\| \leq \eta_k \|\nabla E(z^k)\|, \tag{4.17}$$

where $\eta_k := \min\{\|\nabla E(y^k), \eta\|\}$. If (4.17) or

$$\nabla E(z^k)^T d^k \leq -\eta_k \|d^k\|^2$$

is not satisfied, set $d^k := -B_k^{-1}\nabla E(z^k)$, where matrix B_k is positive definite in $\mathcal{S}^m$.

Step 2. Set $t_k := \sigma^{j_k}$ and $z^{k+1} := z^k + t_k d^k$, where j_k is the smallest nonnegative integer j satisfying

$$E(z^k + \sigma^j d^k) - E(z^k) \le \mu \sigma^j \nabla E(z^k)^T d^k \,.$$

Step 3. Set $k := k+1$ and go to Step 1.

For implementing Algorithm 2, V_k is required at each kth step. Applying the contents in Section 2.2 and Section 2.3 of Chapter 2, we can calculate one element $V_z \in \hat{\partial}^2 E(z)$ as follows.

Denote

$$X(z) := \Pi_{\mathcal{S}^n_+}[X^k - \frac{1}{\alpha}(\nabla f(X^k) - \mathcal{A}^* z)]$$

and

$$\lambda(z) := \lambda(X(z)).$$

Let $X(z)$ admit the spectral decomposition as

$$X(z) = P \mathrm{diag}(\lambda(z)) P^T, \quad P \in \mathcal{O}_{X(z)}.$$

Define three index sets of positive, zero and negative eigenvalues of $\lambda(z)$, respectively, as

$$\alpha^* := \{i : \lambda_i(z) > 0\}, \quad \beta^* := \{i : \lambda_i(z) = 0\}, \quad \gamma^* := \{i : \lambda_i(z) < 0\}.$$

Let $U_z : \mathcal{S}^n \longrightarrow \mathcal{S}^n$ be defined by

$$U_z H = P(W_z \circ (P^T H P))P^T, \quad H \in S^n, \tag{4.18}$$

where

$$W_z := \begin{bmatrix} E_{\alpha^*\alpha^*} & E_{\alpha^*\beta^*} & (v_{ij})_{\substack{i\in\alpha^* \\ j\in\gamma^*}} \\ E^T_{\alpha^*\beta^*} & 0 & 0 \\ (v_{ji})_{\substack{i\in\alpha^* \\ j\in\gamma^*}} & 0 & 0 \end{bmatrix}, \quad v_{ij} = \frac{\lambda_i(z)}{\lambda_i(z) - \lambda_j(z)}, \; i \in \alpha^*, \; j \in \gamma^*.$$

From Pang, Sun and Sun [24], we know that $U_z \in \partial_B \Pi_{\mathcal{S}^n_+}(X(z))$. Then for any $h \in \Re^m$, we can define $V_z : \Re^m \to \Re^m$ by

$$V_z h := \frac{1}{\alpha}\mathcal{A}(U_z(\mathcal{A}^* h)) + \frac{1}{\rho\beta}\begin{bmatrix} 0 \\ h_2 - C_2 h_2 \\ h_3 - C_3 h_3 \\ h_4 - C_4 h_4 \end{bmatrix}$$

$$= \frac{1}{\alpha}\mathcal{A}P(W_z \circ (P^T(\mathcal{A}^* h)P))P^T + \frac{1}{\rho\beta}\begin{bmatrix} 0 \\ h_2 - C_2 h_2 \\ h_3 - C_3 h_3 \\ h_4 - C_4 h_4 \end{bmatrix}, \qquad (4.19)$$

where C_2 is a $q_e \times q_e$ diagonal matrix such that

$$(C_2)_{ii} = \begin{cases} 0, & \text{if} \quad |(r^k)_i - \frac{1}{\rho\beta}(z_2)_i| > \frac{1}{\beta} \\ 1, & \text{if} \quad |(r^k)_i - \frac{1}{\rho\beta}(z_2)_i| \le \frac{1}{\beta}\,, \end{cases} \qquad (4.20)$$

C_3 is a $q_l \times q_l$ diagonal matrix such that

$$(C_3)_{ii} = \begin{cases} 0, & \text{if} \quad |(v^k)_i - \frac{1}{\rho\beta}(z_3)_i| > \frac{1}{\beta} \text{ or } |(v^k)_i - \frac{1}{\rho\beta}(z_3)_i| < 0 \\ 1, & \text{if} \quad 0 \le |(v^k)_i - \frac{1}{\rho\beta}(z_3)_i| \le \frac{1}{\beta} \end{cases} \qquad (4.21)$$

and C_4 is a $q_u \times q_u$ diagonal matrix such that

$$(C_4)_{ii} = \begin{cases} 0, & \text{if} \quad |(w^k)_i - \frac{1}{\rho\beta}(z_4)_i| > \frac{1}{\beta} \text{ or } |(w^k)_i - \frac{1}{\rho\beta}(z_4)_i| < 0 \\ 1, & \text{if} \quad 0 \le |(w^k)_i - \frac{1}{\rho\beta}(z_4)_i| \le \frac{1}{\beta}\,. \end{cases} \qquad (4.22)$$

By applying the results above, we obtain that $V_z h \in \hat{\partial}^2 E(z)h$. In particular, we do not need V_z explicitly in Algorithm 2.

4.3 Convergence analysis

In this section, we focus on the convergence analysis of the semismooth Newton-CG method.

In problem (4.2), the generalized Slater condition (4.12) naturally holds, then the infinite sequence $\{z^k\}$ generated by Algorithm 2 is bounded. Furthermore, this sequence has at least one accumulation point denoted by z^*. Here, z^* is the solution to problem (4.6). By borrowing the convergence results from Qi and Sun [25] and Bai, Chu and Sun [2], we have the following theorem.

Theorem 4.3.1. Suppose that both $\{\|B_k\|\}$ and $\{\|B_k^{-1}\|\}$ in Algorithm 2 are uniformly bounded. Then, any accumulation point z^* of the infinite sequence $\{z^k\}$ generated by Algorithm 2 is a solution to the problem (4.6). Moreover, if every element in $\hat{\partial}^2 E(z^*)$ is positive definite at any z^*, then the infinite sequence $\{z^k\}$ converges to solution z^* of (4.6) quadratically.

In Theorem 4.3.1, the key point is to characterize the positive definiteness of every element in $\hat{\partial}^2 E(z^*)$. Here, we need the concept of constraint nondegeneracy. More details can be found in [5]. To apply the constraint nondegeneracy, we reformulate (4.2) as follows:

$$
\begin{array}{ll}
\min & q(X, r, v, w, t_r, t_v, t_w) \\
\text{s.t.} & \mathcal{A}_1(X) = b_1 \,, \\
& \mathcal{A}_2(X) - b_2 = r \,, \\
& -\mathcal{A}_3(X) - b_3 = v \,, \\
& \mathcal{A}_4(X) - b_4 = w \,, \\
& X \in \mathcal{S}^n_+ \,, \\
& (r, t_r) \in K_r \,, \\
& (v, t_v) \in K_v \,, \\
& (w, t_w) \in K_w \,,
\end{array}
\tag{4.23}
$$

where

$$
\begin{aligned}
& q(X,r,v,w,t_r,t_v,t_w) \\
= \; & \frac{1}{2}\|H\circ(X^k-G)\|_F^2 + \langle H\circ H\circ(X^k-G)\,,\,X-X^k\rangle + \frac{\alpha}{2}\|X-X^k\|_F^2 \\
& +\rho(t_r+\frac{\beta}{2}\|r-r^k\|^2+t_v+\frac{\beta}{2}\|v-v^k\|^2+t_w+\frac{\beta}{2}\|w-w^k\|^2)\,,
\end{aligned}
$$

$$K_r := \{\,(r,t_r)\in\Re^{q_e+1}\mid t_r\geq\|r\|_1\,\}\,,$$

$$K_v := \{\,(v,t_v)\in\Re^{q_l+1}\mid t_v\geq\sum_{(i,j)\in\mathcal{B}_l}\max(v_{ij},0)\,\}$$

and

$$K_w := \{\,(w,t_w)\in\Re^{q_u+1}\mid t_w\geq\sum_{(i,j)\in\mathcal{B}_u}\max(w_{ij},0)\,\}\,.$$

Assume that $\bar z$ is an optimal solution to problem (4.6). By recalling the relationship between primal variables and dual variables, we have

$$\overline{X} = \Pi_{\mathcal{S}^n_+}(X^k-\frac{1}{\alpha}(\nabla f(X^k)-\mathcal{A}^*\bar z))$$

and

$$\bar y := \begin{bmatrix} 0 \\ \bar r \\ \bar v \\ \bar w \end{bmatrix},$$

where

$$
\begin{aligned}
\bar r &= P_{\frac{1}{\beta}\|\cdot\|_1}(r^k-\frac{1}{\rho\beta}\bar z_2) = r^k-\frac{1}{\rho\beta}\bar z_2-\Pi_{[-\frac{1}{\beta},\frac{1}{\beta}]}(r^k-\frac{1}{\rho\beta}\bar z_2)\,,\\
\bar v &= P_{\frac{1}{\beta}\max(\cdot,0)}(v^k-\frac{1}{\rho\beta}\bar z_3) = v^k-\frac{1}{\rho\beta}\bar z_3-\Pi_{[0,\frac{1}{\beta}]}(v^k-\frac{1}{\rho\beta}\bar z_3)
\end{aligned}
$$

and

$$\bar w = P_{\frac{1}{\beta}\max(\cdot,0)}(w^k-\frac{1}{\rho\beta}\bar z_4) = w^k-\frac{1}{\rho\beta}\bar z_4-\Pi_{[0,\frac{1}{\beta}]}(w^k-\frac{1}{\rho\beta}\bar z_4)\,.$$

Obviously, $(\overline{X}, \bar{r}, \bar{v}, \bar{w}, \bar{t_r}, \bar{t_v}, \bar{t_w}, \bar{z})$ is the KKT point to problem (4.23). Then, the constraint nondegeneracy of (4.23) is

$$\begin{bmatrix} \mathcal{A}_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{A}_2 & -I & 0 & 0 & 0 & 0 & 0 \\ -\mathcal{A}_3 & 0 & 0 & -I & 0 & 0 & 0 \\ \mathcal{A}_4 & 0 & 0 & 0 & 0 & -I & 0 \\ I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & I & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I \end{bmatrix} \begin{bmatrix} \mathcal{S}^n \\ \Re^{q_e} \\ \Re \\ \Re^{q_l} \\ \Re \\ \Re^{q_u} \\ \Re \end{bmatrix} + \begin{bmatrix} \{0\}^m \\ \operatorname{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big) \end{bmatrix} = \begin{bmatrix} \Re^m \\ \mathcal{S}^n \\ \Re^{q_e} \\ \Re \\ \Re^{q_l} \\ \Re \\ \Re^{q_u} \\ \Re \end{bmatrix}. \tag{4.24}$$

Equivalently, we can rewrite (4.24) as

$$\begin{bmatrix} \mathcal{A}_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{A}_2 & -I & 0 & 0 & 0 & 0 & 0 \\ -\mathcal{A}_3 & 0 & 0 & -I & 0 & 0 & 0 \\ \mathcal{A}_4 & 0 & 0 & 0 & 0 & -I & 0 \end{bmatrix} \begin{bmatrix} \operatorname{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big) \\ \operatorname{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big) \end{bmatrix} = \begin{bmatrix} \Re^n \\ \Re^{q_e} \\ \Re^{q_l} \\ \Re^{q_u} \end{bmatrix}. \tag{4.25}$$

For any $\bar{r} \in \Re^{q_e}$, we define three index sets, respectively, as

$$I_{rp} := \{\, i \,:\, (\bar{r})_i > 0\,\}, \quad I_{rz} := \{\, i \,:\, (\bar{r})_i \,=\, 0\,\}, \quad I_{rn} := \{\, i \,:\, (\bar{r})_i \,<\, 0\,\}.$$

From [7, Theorem 2.4.9], we can characterize $\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})$ and $\operatorname{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big)$ as

$$\mathcal{T}_{K_r}(\bar{r}, \bar{t_r}) := \{(d, s) \in \Re^{q_e+1} \;\mid\; s \geq \sum_{i \in I_{rp}} d_i - \sum_{i \in I_{rn}} d_i + \sum_{i \in I_{rz}} |d_i| \;\} \tag{4.26}$$

and

$$\operatorname{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big) := \{(d, s) \in \Re^{q_l+1} \;\mid\; s = \sum_{i \in I_{rp}} d_i - \sum_{i \in I_{rn}} d_i \,, d_i = 0, \text{ for } i \in I_{rz}\}. \tag{4.27}$$

Similarly, for any $\bar{v} \in \Re^{q_l}$ and $\bar{w} \in \Re^{q_u}$, we define six index sets, respectively, as

$$I_{vp} := \{\, i \,:\, (\bar{v})_i > 0 \,\}, \quad I_{vz} := \{\, i \,:\, (\bar{v})_i = 0 \,\}, \quad I_{vn} := \{\, i \,:\, (\bar{v})_i < 0 \,\}$$

and

$$I_{wp} := \{\, i \,:\, (\bar{w})_i > 0 \,\}, \quad I_{wz} := \{\, i \,:\, (\bar{w})_i = 0 \,\}, \quad I_{wn} := \{\, i \,:\, (\bar{w})_i < 0 \,\}.$$

Then we can characterize $\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})$, $\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})$, $\text{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big)$ and $\text{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big)$ respectively as

$$\mathcal{T}_{K_v}(\bar{v}, \bar{t_v}) := \{(d, s) \in \Re^{q_l+1} \ \mid \ s \geq \sum_{i \in I_{vp}} d_i + \sum_{i \in I_{vz}} \max(d_i, 0)\}\,, \tag{4.28}$$

$$\mathcal{T}_{K_w}(\bar{w}, \bar{t_w}) := \{(d, s) \in \Re^{q_u+1} \ \mid \ s \geq \sum_{i \in I_{wp}} d_i + \sum_{i \in I_{wz}} \max(d_i, 0)\}\,, \tag{4.29}$$

$$\text{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big) := \{(d, s) \in \Re^{q_l+1} \ \mid s = \sum_{i \in I_{vp}} d_i\,,\ d_i = 0,\ \text{for } i \in I_{vz}\} \tag{4.30}$$

and

$$\text{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big) := \{(d, s) \in \Re^{q_u+1} \ \mid s = \sum_{i \in I_{wp}} d_i\,,\ d_i = 0,\ \text{for } i \in I_{wz}\}\,. \tag{4.31}$$

Let $\lambda_1 \geq \cdots \geq \lambda_n$ be the eigenvalues of $\overline{X}$ being arranged in the non-increasing order. Denote $\zeta := \{i \ \mid \ \lambda_i > 0, \quad i = 1, \cdots, n\}$. Then there exists an orthogonal matrix $P \in \Re^{n \times n}$ such that

$$\overline{X} = P \begin{bmatrix} \Lambda_\zeta & 0 \\ 0 & 0 \end{bmatrix} P^T\,, \tag{4.32}$$

where Λ_ζ is the diagonal matrix whose diagonal entries are λ_i for $i \in \zeta$. Denote $\vartheta := \{1, 2, \cdots, n\} \backslash \zeta$. Let $P := [P_\zeta P_\vartheta]$ with $P_\zeta \in \Re^{n \times |\zeta|}$ and $P_\vartheta \in \Re^{n \times |\vartheta|}$. From [1], we can characterize $\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})$ and $\text{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)$ as

$$\mathcal{T}_{\mathcal{S}^n_+}(\overline{X}) = \{B \in \mathcal{S}^n \ \mid \ P_\vartheta^T B P_\vartheta \in \mathcal{S}^n_+\} \tag{4.33}$$

and

$$\mathrm{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big) = \{B \in \mathcal{S}^n \ \mid \ P_\vartheta^T B P_\vartheta = 0\}. \tag{4.34}$$

With the above preparations given, we first prove the following theorem.

Theorem 4.3.2. Assume that $(\overline{X}, \bar{y}, \bar{t_r}, \bar{t_v}, \bar{t_w}, \bar{z})$ is the KKT point to problem (4.23). Let P be an orthogonal matrix such that $\overline{X}$ has the spectral decomposition as in (4.32). Then the following three conclusions are equivalent:

i) The primal constraint nondegeneracy (4.25) of problem (4.23) holds.

ii) Any element in $\hat{\partial}^2 E(\bar{z})$ is symmetric and positive definite.

iii) $V_{\bar{z}}$ (calculated by the method introduced in section 2) $\in \hat{\partial}^2 E(\bar{z})$ is symmetric and positive definite.

Proof. "i) $\Rightarrow$ ii)" Step 1:

Suppose that V is an arbitrary element in $\hat{\partial}^2 E(\bar{z})$, by applying Proposition 2.4.2 in Chapter 2, we know that any element in $\partial P_{\frac{1}{\beta}\|\cdot\|_1}(r^k - \frac{1}{\rho\beta}\bar{z}_2)$ is symmetric and positive semidefinite, any element in $\partial P_{\frac{1}{\beta}\max(\cdot,0)}(v^k - \frac{1}{\rho\beta}\bar{z}_3)$ is symmetric and positive semidefinite, any element in $\partial P_{\frac{1}{\beta}\max(\cdot,0)}(w^k - \frac{1}{\rho\beta}\bar{z}_4)$ is symmetric and positive semidefinite and any element in $\partial\Pi_{\mathcal{S}^n_+}(\overline{X})$ is symmetric and positive semidefinite, hence, V is symmetric and positive semidefinite.

Step 2:

Since V is an element in $\hat{\partial}^2 E(\bar{z})$, then there exist $W_1 \in \partial\Pi_{\mathcal{S}^n_+}(\overline{X})$, $V_2 \in \partial P_{\frac{1}{\beta}\|\cdot\|_1}(r^k - \frac{1}{\rho\beta}\bar{z}_2)$, $V_3 \in \partial P_{\frac{1}{\beta}\max(\cdot,0)}(v^k - \frac{1}{\rho\beta}\bar{z}_3)$ and $V_4 \in \partial P_{\frac{1}{\beta}\max(\cdot,0)}(w^k - \frac{1}{\rho\beta}\bar{z}_4)$ such that

$$Vh = \frac{1}{\alpha}\mathcal{A}W_1\mathcal{A}^*h + \frac{1}{\rho\beta}V_2h_2 + \frac{1}{\rho\beta}V_3h_3 + \frac{1}{\rho\beta}V_4h_4\,, \text{ for any } \ h \in \Re^m\,. \tag{4.35}$$

Assume that there exits a $d \in \Re^m$ such that $\langle d, Vd \rangle = 0$. On one hand, by applying Proposition 2.4.2 in Chapter 2, we have

$$\langle d\,,\, \mathcal{A}W_1\mathcal{A}^*d\rangle = \langle \mathcal{A}^*d\,,\, W_1\mathcal{A}^*d\rangle \geq \|W_1\mathcal{A}^*d\|^2\,,$$

$$\langle d_2\,,\, V_2d_2\rangle \geq \|V_2d_2\|^2\,,$$

$$\langle d_3\,,\, V_3d_3\rangle \geq \|V_3d_3\|^2$$

and

$$\langle d_4\,,\, V_4d_4\rangle \geq \|V_4d_4\|^2\,,$$

which implies

$$W_1\mathcal{A}^*d = 0\,,$$

$$V_2d_2 = 0\,,$$

$$V_3d_3 = 0$$

and

$$V_4d_4 = 0\,.$$

In addition, by the definition of Jacobian amicability and Proposition 2.3.1 of Chapter 2, it follows that

$$\mathcal{A}^*d \in \big(\mathrm{lin}(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X}))\big)^{\perp}. \tag{4.36}$$

On the other hand, by applying (4.25), for this $d \in \Re^m$, there exist $X_1 \in \mathrm{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)$, $(r_1, t_{r1}) \in \mathrm{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big)$, $(v_1, t_{v1}) \in \mathrm{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big)$ and $(w_1, t_{w1}) \in \mathrm{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big)$ such that

$$\begin{bmatrix} \mathcal{A}_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{A}_2 & -I & 0 & 0 & 0 & 0 & 0 \\ -\mathcal{A}_3 & 0 & 0 & -I & 0 & 0 & 0 \\ \mathcal{A}_4 & 0 & 0 & 0 & 0 & -I & 0 \end{bmatrix} \begin{bmatrix} X_1 \\ r_1 \\ t_{r1} \\ v_1 \\ t_{v1} \\ w_1 \\ t_{w1} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix}. \tag{4.37}$$

Thus, we obtain

$$\begin{cases} d_1 = \mathcal{A}_1(X_1)\,, \\ d_2 = \mathcal{A}_2(X_1) - r_1\,, \\ d_3 = -\mathcal{A}_3(X_1) - v_1\,, \\ d_4 = \mathcal{A}_4(X_1) - w_1\,. \end{cases} \tag{4.38}$$

With the above preparations, by applying (4.36) and (4.38), we have

$$\begin{aligned} &\langle d\,,\, d\rangle \\ =\;& \langle \mathcal{A}_1(X_1)\,,\, d_1\rangle + \langle \mathcal{A}_2(X_1) - r_1\,,\, d_2\rangle + \langle -\mathcal{A}_3(X_1) - v_1\,,\, d_3\rangle + \langle \mathcal{A}_4(X_1) - w_1\,,\, d_4\rangle \\ =\;& \langle \mathcal{A}_1^* d_1\,,\, X_1\rangle + \langle \mathcal{A}_2^* d_2\,,\, X_1\rangle - \langle r_1\,,\, d_2\rangle + \langle -\mathcal{A}_3^* d_3\,,\, X_1\rangle - \langle v_1\,,\, d_3\rangle \\ & + \langle \mathcal{A}_4^* d_4\,,\, X_1\rangle - \langle w_1\,,\, d_4\rangle \\ =\;& \langle \mathcal{A}^* d\,,\, X_1\rangle - \langle r_1\,,\, d_2\rangle - \langle v_1\,,\, d_3\rangle - \langle w_1\,,\, d_4\rangle \\ =\;& -\langle r_1\,,\, d_2\rangle - \langle v_1\,,\, d_3\rangle - \langle w_1\,,\, d_4\rangle\,. \end{aligned} \tag{4.39}$$

Recall the characterization of $\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})$ (4.26) and $\text{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big)$ (4.27), we obtain that

$$(r_1)_i = 0\,, \text{ for any } i \in \{j : \bar{r}_j = 0\}\,.$$

Moreover, by direct calculation, we know that there exists a number $\chi_r \in [0, 1]$, such that

$$(V_2 d_2)_i = \begin{cases} (d_2)_i\,, & \text{if } \bar{r}_i \neq 0 \\ \chi_r (d_2)_i\,, & \text{if } \bar{r}_i = 0\,. \end{cases} \tag{4.40}$$

Since $V_2 d_2 = 0$, it follows that

$$(d_2)_i = 0\,, \text{ for any } i \in \{j : \bar{r}_j \neq 0\}.$$

Hence,

$$\langle r_1\,,\, d_2\rangle = 0\,.$$

Similarly, recall the characterization of $\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})$ (4.28), $\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})$ (4.29), $\text{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big)$ (4.30) and $\text{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big)$ (4.31), we obtain that

$$(v_1)_i = 0\,, \text{ for any } i \in \{j : \bar{v}_j = 0\}$$

and

$$(w_1)_i = 0\,, \text{ for any } i \in \{j : \bar{w}_j = 0\}\,.$$

By direct calculation, we also know that there exist two numbers $\chi_v \in [0,1]$ and $\chi_w \in [0,1]$, such that

$$(V_3 d_3)_i = \begin{cases} (d_3)_i\,, & \text{if} \quad \bar{v}_i \neq 0 \\ \chi_v (d_3)_i\,, & \text{if} \quad \bar{v}_i = 0 \end{cases} \tag{4.41}$$

and

$$(V_4 d_4)_i = \begin{cases} (d_4)_i\,, & \text{if} \quad \bar{w}_i \neq 0 \\ \chi_w (d_4)_i\,, & \text{if} \quad \bar{w}_i = 0\,. \end{cases} \tag{4.42}$$

Since $V_3 d_3 = 0$ and $V_4 d_4 = 0$, it follows that

$$(d_3)_i = 0\,, \text{ for any } i \in \{j : \bar{v}_j \neq 0\}$$

and

$$(d_4)_i = 0\,, \text{ for any } i \in \{j : \bar{w}_j \neq 0\}\,.$$

Hence, we have

$$\langle v_1\,,\, d_3 \rangle = 0$$

and

$$\langle w_1\,,\, d_4 \rangle = 0\,.$$

Therefore, by (4.39), we obtain that

$$\langle d\,,\, d \rangle = 0\,,$$

which implies that $d = 0$. We conclude that the nonsingularity of V holds.

Step 3:

By combining the conclusions in Step 1 and Step 2, we know that V is symmetric and positive definite. The proof is complete. □

"ii) $\Rightarrow$ iii)" It is obviously true since $V_{\bar{z}} \in \hat{\partial}^2 E(\bar{z})$.

"iii) $\Rightarrow$ i)" We prove this conclusion by contradiction. Assume on the contrary that the primal constraint nondegeneracy (4.25) of problem (4.23) does not hold.

Firstly, for simplicity, we denote

$$\mathcal{Z} := \begin{bmatrix} \mathcal{A}_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \mathcal{A}_2 & -I & 0 & 0 & 0 & 0 & 0 \\ -\mathcal{A}_3 & 0 & 0 & -I & 0 & 0 & 0 \\ \mathcal{A}_4 & 0 & 0 & 0 & 0 & -I & 0 \end{bmatrix} \begin{bmatrix} \text{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big) \\ \text{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big) \\ \text{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big) \\ \text{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big) \end{bmatrix}.$$

Then, there exists $0 \neq d \in \Re^m$ such that $d \in \mathcal{Z}^\perp$, namely, there exists $0 \neq d \in \Re^m$ such that, for any $X \in \text{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)$, any $(r, t_r) \in \text{lin}\big(\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})\big)$, any $(v, t_v) \in \text{lin}\big(\mathcal{T}_{K_v}(\bar{v}, \bar{t_v})\big)$ and any $(w, t_w) \in \text{lin}\big(\mathcal{T}_{K_w}(\bar{w}, \bar{t_w})\big)$, we have

$$\left\langle \begin{pmatrix} \mathcal{A}_1(X) \\ \mathcal{A}_2(X) - r \\ -\mathcal{A}_3(X) - v \\ \mathcal{A}_4(X) - w \end{pmatrix}, d \right\rangle = 0, \tag{4.43}$$

which implies

$$\begin{aligned} & \langle \mathcal{A}_1(X), d_1 \rangle + \langle \mathcal{A}_2(X) - r, d_2 \rangle + \langle -\mathcal{A}_3(X) - v, d_3 \rangle + \langle \mathcal{A}_4(X) - w, d_4 \rangle \\ = \; & \langle \mathcal{A}_1^* d_1, X \rangle + \langle \mathcal{A}_2^* d_2, X \rangle - \langle r, d_2 \rangle + \langle -\mathcal{A}_3^* d_3, X \rangle - \langle v, d_3 \rangle \\ & + \langle \mathcal{A}_4^* d_4, X \rangle - \langle w, d_4 \rangle \\ = \; & \langle \mathcal{A}^* d, X \rangle - \langle r, d_2 \rangle - \langle v, d_3 \rangle - \langle w, d_4 \rangle \\ = \; & 0. \end{aligned} \tag{4.44}$$

By noting that $d \in \mathcal{Z}^\perp$, we can set $X = 0$. Then (4.43) reduces to

$$\langle r, d_2 \rangle + \langle v, d_3 \rangle + \langle w, d_2 \rangle = 0,$$

together with (4.44), it follows that

$$\langle \mathcal{A}^* d\,,\, X\rangle = 0\,, \quad \text{for any } X \in \mathrm{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)\,. \tag{4.45}$$

Secondly, recall the characterization of $\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})$ (4.33) and $\mathrm{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)$ (4.34), for any $X \in \mathrm{lin}\big(\mathcal{T}_{\mathcal{S}^n_+}(\overline{X})\big)$, we have

$$\begin{aligned} 0 &= \langle \mathcal{A}^* d\,,\, X\rangle \\ &= \langle P^T \mathcal{A}^* dP\,,\, P^T X P\rangle \\ &= \Big\langle \begin{bmatrix} P_\zeta^T \mathcal{A}^* dP_\zeta & P_\zeta^T \mathcal{A}^* dP_\vartheta \\ P_\vartheta^T \mathcal{A}^* dP_\zeta & P_\vartheta^T \mathcal{A}^* dP_\zeta \end{bmatrix}, \begin{bmatrix} P_\zeta^T X P_\zeta & P_\zeta^T X P_\vartheta \\ P_\vartheta^T X P_\zeta & 0 \end{bmatrix} \Big\rangle. \end{aligned}$$

It follows that

$$P_\zeta^T \mathcal{A}^* dP_\zeta = 0 \tag{4.46}$$

and

$$P_\zeta^T \mathcal{A}^* dP_\vartheta = 0. \tag{4.47}$$

Thirdly, by recalling the definition of $V_{\bar{z}}$ in (4.19), we have

$$\begin{aligned} \langle d\,,\, V_{\bar{z}} d\rangle = {} & \frac{1}{\alpha}\langle d\,,\, \mathcal{A} U_{\bar{z}} \mathcal{A}^* d\rangle + \frac{1}{\rho\beta}\langle d_2\,,\, d_2 - C_2 d_2\rangle \\ & + \frac{1}{\rho\beta}\langle d_3\,,\, d_3 - C_3 d_3\rangle + \frac{1}{\rho\beta}\langle d_4\,,\, d_4 - C_4 d_4\rangle. \end{aligned} \tag{4.48}$$

Denote

$$t_2' := \sum_{i \in I_{rp}} (d_2 - C_2 d_2)_i - \sum_{i \in I_{rn}} (d_2 - C_2 d_2)_i\,.$$

By the characterization of $\mathcal{T}_{K_r}(\bar{r}, \bar{t_r})$ (4.26), we can obtain that

$$(d_2 - C_2 d_2, t_2') \in \mathcal{T}_{K_r}(\bar{r}, \bar{t_r}),$$

which implies that

$$\langle d_2\,,\, d_2 - C_2 d_2\rangle = 0. \tag{4.49}$$

Similarly, denote

$$t_3' := \sum_{i\in I_{rp}} (d_3 - C_3 d_3)_i$$

and

$$t_4' := \sum_{i\in I_{wp}} (d_4 - C_4 d_4)_i\,.$$

By the characterization of $\mathcal{T}_{K_v}(\bar{v},\bar{t_v})$ (4.28) and $\mathcal{T}_{K_w}(\bar{w},\bar{t_w})$ (4.29), we can obtain that

$$(d_3 - C_3 d_3, t_3') \in \mathcal{T}_{K_v}(\bar{v},\bar{t_v})$$

and

$$(d_4 - C_4 d_4, t_4') \in \mathcal{T}_{K_w}(\bar{w},\bar{t_w})\,,$$

which implies that

$$\langle d_3\,,\, d_3 - C_3 d_3\rangle = 0 \tag{4.50}$$

and

$$\langle d_4\,,\, d_4 - C_4 d_4\rangle = 0. \tag{4.51}$$

Moreover, by applying (4.46) and (4.47), we obtain that

$$\begin{aligned}
&\langle d\,,\, \mathcal{A}U_{\bar z}\mathcal{A}^* d\rangle\\
=\;&\langle \mathcal{A}^* d\,,\, U_{\bar z}\mathcal{A}^* d\rangle\\
=\;&\langle P^T\mathcal{A}^* dP\,,\, W_{\bar z}\circ(P^T\mathcal{A}^* dP)\rangle\\
=\;&\langle \begin{bmatrix} 0 & 0\\ 0 & Q\end{bmatrix}, \begin{bmatrix} E_{\zeta\zeta} & \Omega_{12}\\ \Omega_{12}^T & 0\end{bmatrix}\circ\begin{bmatrix} 0 & 0\\ 0 & Q\end{bmatrix}\rangle\\
=\;&0\,,
\end{aligned} \tag{4.52}$$

where $Q \in \Re^{|\vartheta|\times|\vartheta|}$ and $\Omega_{12} \in \Re^{|\zeta|\times|\vartheta|}$.

Finally, by combining (4.48), (4.49), (4.50), (4.51) and (4.52), we obtain

$$\langle d\,,\, V_{\bar z} d\rangle = 0\,,$$

which contradicts with the positive definiteness of $V_{\bar{z}}$. This completes the proof.

Now, we are ready to prove the convergence result of Algorithm 2 which is similar to Theorem 3.5 in [26].

Theorem 4.3.3. Let the sequence $\{z^k\}$ be generated by Algorithm 2 which is applied to solve the problem (4.6). Assume that both $\{\|B_k\|\}$ and $\{\|B_k^{-1}\|\}$ in Algorithm 2 are uniformly bounded. If the primal constraint nondegeneracy (4.25) of problem (4.23) holds at the accumulation point of the sequence $\{z^k\}$, then the whole sequence $\{z^k\}$ quadratically converges to the unique solution of (4.6).

Proof. Firstly, since the generalized Slater's condition (4.12) of problem (4.2) naturally holds, then the sequence $\{z^k\}$ is bounded and has at least one accumulation point which is denoted by z^*. Furthermore, by applying Theorem 4.3.1, we know that the accumulation point z^* solves the optimization problem (4.6), i.e., it is an optimal solution to problem (4.6). Finally, since the primal constraint nondegeneracy (4.25) of problem (4.23) holds at z^*, by applying Theorem 4.3.1 and Theorem 4.3.2, it follows that the whole sequence $\{z^k\}$ quadratically converges to z^*. This completes the proof. □

Chapter 5

Numerical Experiments

5.1 Implementation issues

In this section, we address several practical issues in the numerical implementation for solving the problem (1.3).

i) CG in Newton's method.

To solve (4.16) more efficiently, we need a proper preconditioner to apply PCG method instead of CG method. In our numerical implementation, we borrow the essential idea developed in [9, 39] to design an approximate diagonal preconditioner. We denote by A the matrix representation of $\mathcal{A}$ defined in (1.4) with respect to the standard basis in $\mathcal{S}^n$ and U_M the matrix representation of U_z defined in (4.18) with respect to the standard basis in $\Re^m$. Then the coefficient matrix in (4.16) can be represented as AU_MA^T. By noting that the special structure of $\mathcal{A}$, we can easily compute

$$d_{(i,j)} := ((P \circ P)W_z(P \circ P)^T))_{(i,j)}, \quad \text{for } 1 \leq i \leq j \leq n \,,$$

where W_z and P are defined in (4.18). Thus we simply use $\text{diag}(A(\text{Diag}(d))A^T)$

as our diagonal preconditioner for AU_MA^T. Numerical results indicate that this preconditioner works well.

Besides (4.16), we have another choice to calculate the Newton direction, i.e., we apply the PCG method to the following perturbed Newton equation:

$$\nabla E(z^k) + (V_k + \epsilon_k I)d = 0\,, \tag{5.1}$$

where $\varepsilon_k = \min(10^{-3}, 0.1\|\nabla E(z^k)\|)$. Since V_k is positive semidefinite for each $k \geq 0$, then the matrix $(V_k + \epsilon_k I)$ is also positive definite for each $k \geq 0$.

ii) The stopping criterion.

We terminate Algorithm 2 if $\|\nabla_z E(z)\| < 10^{-5}$. Moreover, we terminate Algorithm 1 if

$$\frac{\|X^{k+1} - X^k\|_F}{\max(\|X^k\|_F, 1)} < \text{tol}$$

and

$$\frac{\|y^{k+1} - y^k\|}{\max(\|y^k\|, 1)} < \text{tol}\,,$$

where tol $= 10^{-4}$. Finally, we let Cont denote the total number of constraints and Con1 denote the number of the constraints which the solution satisfies. Once ρ is updated, we let Con2 denote the number of the constraints which the later solution satisfies. We terminate the whole algorithm if

$$\frac{|\text{Con1} - \text{Con2}|}{|\text{Cont}|} \leq \text{ra} \quad \text{or} \quad \rho > 2000\,.$$

where ra $= 0.01\%$. Actually, other stopping criterion can also be used. For example, we can terminate the whole algorithm if

$$|\text{Con1} - \text{Con2}| = 0 \quad \text{or} \quad \rho > 2000\,.$$

It depends on the practical need.

To achieve a faster convergence rate, we apply a so-called continuation technique in our numerical implementation. Generally speaking, at the first step of the majorization method, we set a tolerance for the inner problem in advance; later, for any $k \geq 1$, we introduce a parameter called CT^k and input $\min(\mathrm{CT}^k \times \|\nabla_{z^k} E(z^k)\|, 10^{-5})$ as a tolerance for the inner problem at the (k+1)th step. Hence, we can balance the accuracy between outer problem and inner problem.

iii) Parameters and settings.

In our numerical implementation, we set the Lipschitz constant α as the maximum value in the matrix $H \circ H$. Let $\beta = 0.005$, $\eta = 0.01$, $\mu = 10^{-4}$ and $\sigma = 0.5$. We choose the initial penalty parameter ρ to be 10 and update it by multiplying 5. In fact, the users can choose the other initial value of ρ and increase ρ by multiplying other factors. It depends on the practical need. For simplicity, we fix $B_k = I$ for all $k > 0$. We start from the initial points as $X = G$, $r = 0$, $v = 0$, $w = 0$. We define the ratio as $\mathrm{prob}_e := \frac{2q_e}{n(n-1)}$, $\mathrm{prob}_l := \frac{2q_l}{n(n-1)}$ and $\mathrm{prob}_u := \frac{2q_u}{n(n-1)}$ respectively.

5.2 Numerical results

In this section, we report our numerical results. The numerical experiments are performed on CPU of Core Duo 2.26 GHz and RAM of 4.00 GB. The version of matlab is 7.9.0. The testing examples are given blow.

Example 5.2.1 We set the ratio $\mathrm{prob}_e = [0.001, 0.01, 0.1, 0.3]$, $\mathrm{prob}_l = 0.1$ and $\mathrm{prob}_u = 0.1$ respectively. We take $l_{ij} = -0.3$ for $(i,j) \in \mathcal{B}_l$ and $u_{ij} = 0.3$ for $(i,j) \in \mathcal{B}_u$. e_{ij} is randomly generated with all entries uniformly distributed in [-0.3, 0.3]. The weight matrix H is randomly generated with all entries uniformly distributed in [0.1, 1]. The correlation matrix G is the 387×387 1-day correlation matrix from RiskMetrics(15 June 2006). For testing purposes we set G as

$$G := 0.9G + 0.1C\,,$$

where C is a randomly generated symmetric matrix with entries in $[-1, 1]$.The matlab code is load x.mat; G = subtract(x); C = 2*rand(387)-1; C = (C + C')/2; G = 0.9 *G + 0.1 *C; G = G -diag(diag(G)) + eye(387).

Example 5.2.2 We set $n = [500, 1000]$ and the ratio $\text{prob}_e = [0.001, 0.01, 0.1, 0.3]$, $\text{prob}_l = 0.1$ and $\text{prob}_u = 0.1$ respectively. We take $e_{ij} = G_{ij}$, $l_{ij} = -0.3$ for $(i, j) \in \mathcal{B}_l$ and $u_{ij} = 0.3$ for $(i, j) \in \mathcal{B}_u$. The weight matrix H is generated in the same way as in Example 5.2.1. A correlation matrix G is first generated by using MATLAB's built-in function "randcorr". Then we set G as

$$G := 0.9G + 0.1C\,,$$

where C is s randomly generated symmetric matrix with entries in $[-1, 1]$. The matlab code is x = 10.ˆ [-4:4/(n-1):0]; G = gallery('randcorr',n*x/sum(x)); C = 2*rand(n)-1; C = (C + C')/2; G = 0.9*G + 0.1*C; G = G - diag(diag(G)) + eye(n).

Example 5.2.3 We set $n = [500, 1000]$ and the ratio $\text{prob}_e = [0.001, 0.01, 0.1]$, $\text{prob}_l = 0.1$ and $\text{prob}_u = 0.1$ respectively. We take $l_{ij} = -0.3$ for $(i, j) \in \mathcal{B}_l$ and $u_{ij} = 0.3$ for $(i, j) \in \mathcal{B}_u$. e_{ij} is randomly generated with all entries uniformly distributed in [-0.3, 0.3]. The weight matrix H is generated in the same way as in Example 5.2.1. G is a randomly generated symmetric matrix with $G_{ij} \in [-1, 1]$ and $G_{ii} = 1.0$, $i, j = 1, 2, \cdots, n$. The matlab code is G = 2* rand(n) -1; G = (G + G')/2 - diag(diag(G)) + eye(n).

Example 5.2.4 All the data are the same as in Example 5.2.1 except that we set $e_{ij} = G_{ij}$ and $\text{prob}_e = [0.001, 0.01, 0.1]$.

Example 5.2.5 All the data are the same as in Example 5.2.2 except that e_{ij} is randomly generated with all entries uniformly distributed in [-0.3, 0.3] and $\text{prob}_e = [0.001, 0.01, 0.1]$.

Example 5.2.6 All the data are the same as in Example 5.2.3 except that we set $e_{ij} = G_{ij}$.

Our numerical results are reported in Tables 5.1–5.6. "Ratio" stands for the ratio of the constraints which the solution satisfies. "Time" stands for the total computing time measured in seconds. "Hard.inf" stands for the hard infeasibility measured by $\|\text{diag}(I) - \text{diag}(X)\|_\infty$. "Soft.fix" stands for the soft infeasibility od $r_{ij}, (i, j) \in \mathcal{B}_e$ measured by $\|r\|_\infty$. "Soft.low" stands for the soft infeasibility of $v_{ij}, (i, j) \in \mathcal{B}_l$ measured by $\min(-v_{ij})$, for $(i, j) \in \mathcal{B}_l$. "Soft.upp" stands for the soft infeasibility of $w_{ij}, (i, j) \in \mathcal{B}_u$ measured by $\max(w_{ij})$, for $(i, j) \in \mathcal{B}_u$.

From the numerical results reported in Tables 5.1–5.6, we can see that our algorithm achieves a decent accuracy on hard infeasibility and soft infeasibility simultaneously if the problem is feasible. The soft infeasibility decreases and the "Ratio" increases along with the increase of ρ. If the problem is infeasible, our algorithm also achieves a decent accuracy on the hard infeasibility. To some degree, our algorithm adjusts the value of "Ratio" and the soft infeasibility by increasing the value of ρ. In another word, we achieve a relatively approximate solution after our algorithm terminates. All the tested examples show that our algorithm is efficient and robust.

Table 5.1: Testing results for Example 5.2.1

prob_e	(ρ,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
0.001	(10,99.98%)	104.9	5.326e-07	4.040e-02	-1.454e-07	1.919e-07
	(50,100%)	18.79	7.163e-07	1.876e-06	-1.076e-07	5.701e-07
0.01	(10,99.94%)	116.4	3.341e-07	2.286e-01	-7.608e-08	1.418e-07
	(50,100%)	53.66	9.497e-07	1.066e-06	-1.392e-07	3.708e-07
0.1	(10,99.94%)	105.2	2.123e-07	1.398e-01	-3.874e-08	3.982e-08
	(50,100%)	40.00	4.640e-07	3.972e-07	-6.028e-08	7.677e-08
0.3	(10,72.07%)	188.4	2.784e-09	4.261e-01	-5.340e-10	4.194e-10
	(50,72.31%)	268.7	4.879e-08	4.308e-01	-6.333e-10	1.296e-08
	(250,72.40%)	446.8	1.558e-07	4.309e-01	2.684e-08	-3.004e-09
	(1250,72.41%)	1943	7.084e-09	4.309e-01	-1.230e-09	9.272e-10

Table 5.2: Testing results for Example 5.2.2

(prob_e,n)	(ρ,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
(0.001,500)	(10,100%)	76.88	5.949e-08	5.207e-08	4.483e-02	-4.156e-02
(0.01,500)	(10,100%)	72.19	1.774e-08	1.006e-08	-2.297e-09	-3.397e-03
(0.1,500)	(10,100%)	88.96	5.355e-08	5.909e-08	3.831e-02	-3.232e-02
(0.3,500)	(10,100%)	152.3	3.594e-07	1.024e-07	2.397e-03	-4.426e-02
(0.001,1000)	(10,100%)	539.6	6.110e-08	2.949e-08	8.180e-02	-9.463e-02
(0.01,1000)	(10,100%)	498.5	3.212e-08	1.361e-08	9.773e-02	-8.888e-02
(0.1,1000)	(10,100%)	669.1	4.520e-08	1.405e-08	1.034e-01	-8.734e-02
(0.3,1000)	(10,100%)	1163	4.790e-07	1.032e-07	1.136e-01	-1.267e-01

Table 5.3: Testing results for Example 5.2.3

(prob_e,n)	$(\rho$,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
(0.001,500)	(10,100%)	90.92	9.630e-08	7.107e-08	-3.881e-08	5.852e-08
(0.01,500)	(10,100%)	84.26	1.235e-07	7.446e-08	-2.373e-08	2.357e-08
(0.1,500)	(10,99.99%)	189.0	2.464e-07	3.999e-03	-4.996e-08	6.210e-09
	(50,100%)	195.2	1.293e-07	5.159e-08	-7.585e-09	1.179e-08
(0.001,1000)	(10,100%)	546.0	8.380e-08	1.037e-07	-2.036e-08	2.386e-08
(0.01,1000)	(10,100%)	826.1	3.090e-07	1.163e-07	-3.806e-08	2.451e-08

Table 5.4: Testing results for Example 5.2.4

prob_e	$(\rho$,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
0.001	(10, 100%)	117.0	5.413e-07	3.961e-07	-8.907e-08	2.072e-07
0.01	(10, 99.95%)	126.9	4.449e-07	1.191e-01	-7.024e-08	3.125e-07
	(50, 99.99%)	96.15	7.759e-07	4.701e-02	-1.771e-07	3.253e-07
	(250, 99.99%)	121.4	5.847e-07	4.268e-02	-1.179e-07	2.636e-07
0.1	(10, 94.67%)	212.9	3.793e-07	4.798e-01	-2.358e-02	3.403e-01
	(50, 95.34%)	294.2	8.316e-09	4.731e-01	-9.080e-03	3.232e-01
	(250, 95.45%)	517.0	5.706e-09	4.757e-01	-8.788e-05	3.155e-01
	(1250, 95.45%)	1614	7.551e-09	4.783e-01	-3.034e-09	3.144e-01

Table 5.5: Testing results for Example 5.2.5

(prob_e,n)	(ρ,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
(0.001,500)	(10,100%)	83.92	7.470e-08	5.425e-08	3.067e-09	-8.153e-03
(0.01,500)	(10,100%)	108.8	4.354e-08	4.943e-08	5.048e-02	4.025e-09
(0.1,500)	(10,100%)	191.6	4.533e-07	7.801e-08	7.374e-02	-5.836e-02
(0.001,1000)	(10,100%)	486.0	8.210e-08	4.330e-08	8.723e-02	-8.577e-02
(0.01,1000)	(10,100%)	631.7	1.312e-07	1.149e-07	9.354e-02	-1.063e-01

Table 5.6: Testing results for Example 5.2.6

(prob_e,n)	(ρ,Ratio)	Time	Hard.inf	Soft.fix	Soft.low	Soft.upp
(0.001,500)	(10,100%)	149.6	5.654e-07	3.369e-07	-1.426e-07	1.792e-07
(0.01,500)	(10,99.85%)	208.5	2.884e-07	2.754e-01	-5.863e-08	5.941e-08
	(50,99.97%)	440.0	6.152e-07	2.176e-01	-2.373e-07	1.167e-07
	(250,99.97%)	731.4	9.454e-07	2.152e-01	-2.393e-07	1.448e-07
(0.1,500)	(10,80.91%)	122.8	3.297e-07	9.502e-01	-8.738e-08	7.569e-08
	(50,81.40%)	227.3	5.097e-09	9.617e-01	-1.505e-09	1.231e-09
	(250,81.52%)	349.5	3.705e-09	9.811e-01	-1.759e-09	1.315e-09
	(1250,81.52%)	1054	4.748e-09	9.852e-01	-1.831e-09	1.694e-09
(0.001,1000)	(10,99.99%)	1438	5.209e-07	1.011e-01	-1.734e-07	1.859e-07
	(50,100%)	713.0	1.017e-06	1.665e-06	-8.501e-08	4.042e-08

Chapter 6

Conclusions

In this thesis, we applied the essential idea of the exact penalty method to solve the problem (1.2), i.e., we consider the following penalized problem:

$$\begin{array}{ll} \min & F_\rho(X, r, v, w) \\ \text{s.t.} & X_{ii} = 1\,, \quad i = 1, 2, \ldots, n\,, \\ & X_{ij} - e_{ij} = r_{ij}\,, \quad (i,j) \in \mathcal{B}_e\,, \\ & l_{ij} - X_{ij} = v_{ij}\,, \quad (i,j) \in \mathcal{B}_l\,, \\ & X_{ij} - u_{ij} = w_{ij}\,, \quad (i,j) \in \mathcal{B}_u\,, \\ & X \in \mathcal{S}^n_+\,, \end{array} \tag{6.1}$$

where

$$F_\rho(X, r, v, w) := \frac{1}{2}\|H \circ (X - G)\|_F^2 + \rho\Big(\sum_{(i,j)\in\mathcal{B}_e} |r_{ij}| + \sum_{(i,j)\in\mathcal{B}_l} \max(v_{ij}, 0) + \sum_{(i,j)\in\mathcal{B}_u} \max(w_{ij}, 0)\Big)$$

and $\rho > 0$ is a given penalty parameter that decides the allocated weight to the prescribed constraints in the objective function.

Initially, we applied the idea of majorization method to deal with (6.1) by solving a sequence of unconstrained inner problems iteratively. Moreover, we analyzed the convergence to ensure the efficiency of our majorization method. Secondly, based on the metric projection and the Moreau-Yosida regularization, we derived out the inner problem by the Lagrangian dual approach. Furthermore, we took advantage of the strongly semismooth to overcome the difficulty that the objective function in inner problem was not twice continuously differentiable. Then we proposed a semismooth Newton-CG method to solve the inner problem. Finally, we analyzed the convergence properties of our semismooth Newton-CG method by the using constraint nondegeneracy. The numerical results were reported and showed that our method was efficient and robust.

Our method opens up a way to deal with the problem (1.2) even if it may become infeasible. Some interesting questions in this aspect are worth further study. For example, how do the practitioners identify the constraints which are hard to satisfy and further deal with them according to the different practical need? These questions are left for future research.

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Abstract

In this thesis, we apply the penalty technique to solve the nearest correlation matrix problem, i.e, we consider the penalized version of the former problem. To deal with the penalized problem, we first apply the essential idea of the majorization method by solving a sequence of unconstrained inner problems iteratively. Actually, the inner problem is generated by the Lagrangian dual approach based on the metric projection and the Moreau-Yosida regularization. Since the objective function in the inner problem is not twice continuously differentiable, we take advantage of the strongly semismooth to overcome this difficulty. Then we propose a semismooth Newton-CG method to solve the inner problem. Finally, we analyze the convergence properties of the semismooth Newton-CG method by using the constraint nondegeneracy. The numerical results reported indicate that our algorithm is efficient and robust.

Keywords:
nearest correlation matrix, majorization method, semismoothness, Newton's method

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