Inverse Quadratic Eigenvalue Problems

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July 16, 2006 This talk is based on a joint work with Zheng-Jian Bai and <u>Delin Chu</u> Given $A \in S^n$ (the space of real symmetric matrices of order n), how can we find a positive semidefinite (PSD) matrix $X \in S^n_+$ such that $||X - A||_F$ is minimized?

Mathematically,

$$X \in \operatorname{argmin} \quad \frac{1}{2} \langle X - A, X - A \rangle_F$$

s.t. $X \succeq 0$.

The answer is straightforward. Let \mathcal{O}^n denote the set of all orthonormal matrices in $\mathbb{R}^{n \times n}$. Let $P \in \mathcal{O}^n$ be such that

$$A = P \operatorname{diag}(\sigma_1(A), \sigma_2(A), \cdots, \sigma_n(A)) P^T.$$

Then the unique solution, A_+ , which is actually the metric projection of A onto S_+^n , is given by [Higham'88, Tseng'98]

Pdiag $((\sigma_1(A))_+, (\sigma_2(A))_+, \cdots, (\sigma_n(A))_+)P^T$.

For given $M, C, K \in \mathbb{R}^{n \times n}$, let

$$Q(\lambda) := \lambda^2 M + \lambda C + K.$$

Then the quadratic eigenvalue problem (QEP) is to find scalars $\lambda \in \mathbb{C}$ and nonzero vectors **x** such that

$$Q(\lambda)\mathbf{x} = 0.$$

where λ and **x** are called the eigenvalue and the eigenvector, respectively.

The general Inverse QEP (IQEP) can be defined as follows:

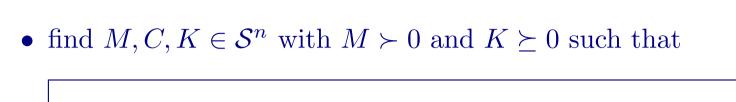
• Given a measured partial eigenpair $(\Lambda, X) \in \mathbb{R}^{k \times k} \times \mathbb{R}^{n \times k}$ with $1 \le k \le n$, $\operatorname{rank}(X) = k$,

$$\Lambda = \operatorname{diag}\{\Lambda_1, \ldots, \Lambda_{\mu}, \Lambda_{\mu+1}, \ldots, \Lambda_{\nu}\},\$$

$$\Lambda_{i} = \operatorname{diag}\{\overbrace{\lambda_{i}^{[2]}, \dots, \lambda_{i}^{[2]}}^{s_{i}}\} \quad \text{for} \quad 1 \leq i \leq \mu,$$
$$\Lambda_{i} = \lambda_{i}I_{s_{i}} \quad \text{for} \quad \mu + 1 \leq i \leq \nu,$$

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$$\begin{split} \lambda_i^{[2]} &= \begin{bmatrix} \alpha_i & \beta_i \\ -\beta_i & \alpha_i \end{bmatrix} \in \mathbb{R}^{2 \times 2}, \quad \beta_i \neq 0, \\ \sigma(\Lambda_i) \cap \sigma(\Lambda_j) &= \emptyset, \quad \forall 1 \le i \ne j \le \mu, \\ \lambda_i \in \mathbb{R}, \quad \lambda_i \ne \lambda_j, \quad \forall \mu + 1 \le i \ne j \le \nu, \end{split}$$



$$MX\Lambda^2 + CX\Lambda + KX = 0.$$

M. Chu, Kuo, and Lin (2004) showed that the general IQEP admits a nontrivial solution, i.e, there exist

> $M \succ 0, C = C^T, K \succeq 0$ satisfying $MX\Lambda^2 + CX\Lambda + KX = 0.$

For given $M_a, C_a, K_a \in S^n$, which are called the estimated analytic <u>mass</u>, damping, and <u>stiffness</u> matrix, the IQEP is

inf
$$\frac{c_1}{2} \|M - M_a\|^2 + \frac{c_2}{2} \|C - C_a\|^2 + \frac{1}{2} \|K - K_a\|^2$$

s.t.
$$MX\Lambda^2 + CX\Lambda + KX = 0$$
,

$$M \succ 0 (M \succeq 0), \quad C = C^T, \quad K \succeq 0,$$

where $c_1 > 0$ and $c_2 > 0$.

Let the QR factorization of X be given by

$$X = Q \begin{bmatrix} R \\ 0 \end{bmatrix},$$

where $Q \in \mathbb{R}^{n \times n}$ is orthogonal and $R \in \mathbb{R}^{k \times k}$ is nonsingular and upper triangular.

By doing variables substitution,

$$M := \sqrt{c_1} Q^T M Q, M_a := \sqrt{c_1} Q^T M_a Q, etc.$$

The IQEP becomes $\min \quad \frac{1}{2} \|M - M_a\|^2 + \frac{1}{2} \|C - C_a\|^2 + \frac{1}{2} \|K - K_a\|^2$ s.t. $\frac{1}{\sqrt{c_1}}M \begin{vmatrix} R \\ 0 \end{vmatrix} \Lambda^2 + \frac{1}{\sqrt{c_2}}C \begin{vmatrix} R \\ 0 \end{vmatrix} \Lambda + K \begin{vmatrix} R \\ 0 \end{vmatrix} = 0,$ $(M, C, K) \in \Omega,$ where $\Omega_0 := \mathcal{S}^n \times \mathcal{S}^n \times \mathcal{S}^n$ $\Omega := \{ (M, C, K) \in \Omega_0 : M \succeq 0, \quad K \succeq 0 \}.$

Theorem 1. The IQEP has a strictly feasible solution iff

 $Det(\Lambda) \neq 0.$

Remark: If $Det(\Lambda) = 0$, we do not lose generality as we can reduce the IQEP to another problem with a strictly feasible solution.

The IQEP is a special case of

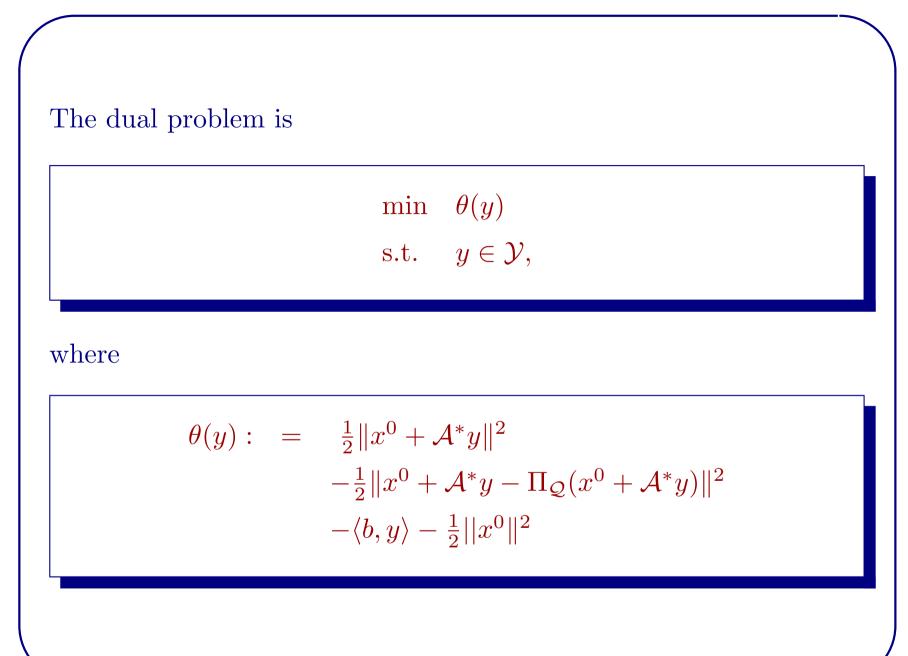
$$\min \quad \frac{1}{2} \langle x - x^0, x - x^0 \rangle$$

s.t. $\mathcal{A}x = b,$
 $x \in \mathcal{Q},$

where $x^0 \in \mathcal{X}, A : \mathcal{X} \to \mathcal{Y}$ is a linear operator, $b \in \mathcal{Y}, \mathcal{Q}$ is a closed convex cone in \mathcal{X} , and \mathcal{X} and \mathcal{Y} are finite dimensional real vector spaces each equipped with a scalar inner product $\langle \cdot, \cdot \rangle$ and its induced norm $\|\cdot\|$. Let $\mathcal{A}^* : \mathcal{Y} \to \mathcal{X}$ be the adjoint of \mathcal{A} . Let $\mathcal{D} \subseteq \mathcal{X}$ be a closed convex set. For any $x \in \mathcal{X}$, let $\Pi_{\mathcal{D}}(x)$ denote the metric projection of x onto \mathcal{D} ,

$$\min \quad \frac{1}{2} \langle z - x, z - x \rangle$$

s.t. $z \in \mathcal{D}$.



and if \mathcal{Q} is a closed convex cone

$$\theta(y) = \frac{1}{2} \|\Pi_{\mathcal{Q}}(x^0 + \mathcal{A}^* y)\|^2 - \langle b, y \rangle - \frac{1}{2} ||x^0||^2.$$

Consider the following equation:

$$F(y) := \nabla \theta(y) = \mathcal{A} \prod_{\mathcal{Q}} (x^0 + \mathcal{A}^* y) - b = 0, \quad y \in \mathcal{Y}.$$

Under Slater's condition

 $\begin{cases} \mathcal{A}: \mathcal{X} \to \mathcal{Y} \text{ is onto,} \\ \exists \ \bar{x} \in \mathcal{X} \text{ such that } \mathcal{A}\bar{x} = b, \ \bar{x} \in \operatorname{int}(\mathcal{Q}), \end{cases}$

where "int" denotes the topological interior, the classical duality theorem [Rockafellar'74] says that

 $x^* := \Pi_{\mathcal{Q}}(x^0 + \mathcal{A}^* y^*)$ solves the original problem if y^* solves $F(y^*) = 0.$

Let \mathcal{Z} be an arbitrary finite dimensional real vector space.

Let \mathcal{O} be an open set in \mathcal{Y} and $\Xi : \mathcal{O} \subseteq \mathcal{Y} \to \mathcal{Z}$ be a locally Lipschitz continuous function on the open set \mathcal{O} .

Rademacher's theorem says that Ξ is almost everywhere Fréchet differentiable in \mathcal{O} .

We denote by \mathcal{O}_{Ξ} the set of points in \mathcal{O} where Ξ is Fréchet differentiable.

Let $\Xi'(y)$ denote the Jacobian of Ξ at $y \in \mathcal{O}_{\Xi}$.

Then Clarke's generalized Jacobian of Ξ at $y\in \mathcal{O}$ is defined by [Clarke'83]

$$\partial \Xi(y) := \operatorname{conv} \{ \partial_B \Xi(y) \},$$

where "conv" denotes the convex hull and

$$\partial_B \Xi(y) := \left\{ V : V = \lim_{j \to \infty} \Xi'(y^j), y^j \to y, y^j \in \mathcal{O}_\Xi \right\}.$$

When $F : \mathcal{O} \subseteq \mathcal{Y} \to \mathcal{Y}$ is continuously differentiable (smooth), the most effective approach for solving

$$F(y) = 0$$

is probably Newton's method. For example, in 1987, S. Smale wrote

If any algorithm has proved itself for the problem of nonlinear systems, it is Newton's method and its many modifications. ... Thus a relation between the simplex method of linear programming and Newton's method, is no surprise. ..." The extension of Newton's methods to Lipschitz systems:

- Friedland, Nocedal, and Overton [87] for inverse eigenvalue problems.
- Kojima and Shindoh [86] for piecewise smooth equations.
- Kummer [88] proposed a condition

(ii) for any $x \to y$ and $V \in \partial \Xi(x)$,

$$\Xi(x) - \Xi(y) - V(x - y) = o(||x - y||).$$

• Finally, Qi and J. Sun [93] showed what needed is <u>semismoothness</u>.

The function Ξ is (strongly) *semismooth* at a point $y \in \mathcal{O}$ if

(i) Ξ is directionally differentiable at y; and

(ii) for any $x \to y$ and $V \in \partial \Xi(x)$,

$$\Xi(x) - \Xi(y) - V(x - y) = o(||x - y||) \ (O(||x - y||^2))$$

Condition (ii) can be replaced by

(ii)' for any $x \to y$ and $x \in \mathcal{O}_{\Xi}$, $\Xi(x) - \Xi(y) - \Xi'(x)(x - y) = o(||x - y||) \ (O(||x - y||^2)).$ Let $A \in S^n$. Then A admits the following spectral decomposition

$$A = P\Sigma P^T,$$

where Σ is the diagonal matrix of eigenvalues of A and P is a corresponding orthogonal matrix of orthonormal eigenvectors.

Define three index sets of positive, zero, and negative eigenvalues of A, respectively, as

$$\alpha := \{i : \sigma_i > 0\},\$$

$$\beta := \{i : \sigma_i = 0\},\$$

$$\gamma := \{i : \sigma_i < 0\}.$$

Write

$$\Sigma = \begin{bmatrix} \Sigma_{\alpha} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Sigma_{\gamma} \end{bmatrix} \text{ and } P = \begin{bmatrix} P_{\alpha} & P_{\beta} & P_{\gamma} \end{bmatrix}$$

with $P_{\alpha} \in \mathbb{R}^{n \times |\alpha|}$, $P_{\beta} \in \mathbb{R}^{n \times |\beta|}$, and $P_{\gamma} \in \mathbb{R}^{n \times |\gamma|}$.

Define the matrix $U \in \mathcal{S}^n$ with entries

$$U_{ij} := \frac{\max\{\sigma_i, 0\} + \max\{\sigma_j, 0\}}{|\sigma_i| + |\sigma_j|}, \quad i, j = 1, \dots, n,$$

where 0/0 is defined to be 1.

Sun and J. Sun [02] showed $\Pi_{\mathcal{S}^n_+}(\cdot)$ is <u>strongly</u> <u>semismooth</u> everywhere and the directional derivative $\Pi'_{\mathcal{S}^n_+}(A; H)$ is given by

	$P_{\alpha}^{T}HP_{\alpha}$	$P_{\alpha}^{T}HP_{\beta}$	$U_{\alpha\gamma} \circ P_{\alpha}^T H P_{\gamma}$	
P	$P_{\beta}^{T}HP_{lpha}$	$\Pi_{\mathcal{S}_{+}^{ \beta }}\left(P_{\beta}^{T}HP_{\beta}\right)$	0	P^T ,
	$P_{\gamma}^{T}HP_{\alpha} \circ U_{\alpha\gamma}^{T}$	0	0	

where \circ denotes the Hadamard product.

When A is nonsingular, i.e., $|\beta| = 0$, $\Pi_{\mathcal{S}^n_+}(\cdot)$ is continuously differentiable around A and the above formula reduces to the classical result of Löwner [34].

The tangent cone of \mathcal{S}^n_+ at $A_+ = \prod_{\mathcal{S}^n_+} (A)$:

$$\mathcal{T}_{\mathcal{S}^n_+}(A_+) = \{ B \in \mathcal{S}^P : P^T_{\bar{\alpha}} B P_{\bar{\alpha}} \succeq 0 \}$$

and the lineality space of $\mathcal{T}_{\mathcal{S}^n_+}(A_+)$, i.e., the largest linear space in $\mathcal{T}_{\mathcal{S}^n_+}(A_+)$,

$$\lim \left(\mathcal{T}_{\mathcal{S}^n_+}(A_+) \right) = \{ B \in \mathcal{S}^n : P^T_{\bar{\alpha}} B P_{\bar{\alpha}} = 0 \},$$

where $\bar{\alpha} := \{1, \ldots, n\} \setminus \alpha$ and $P_{\bar{\alpha}} := [P_{\beta} P_{\gamma}].$

Let W(H) be defined by

$$P \begin{bmatrix} P_{\alpha}^{T} H P_{\alpha} & P_{\alpha}^{T} H P_{\beta} & U_{\alpha\gamma} \circ P_{\alpha}^{T} H P_{\gamma} \\ P_{\beta}^{T} H P_{\alpha}^{T} & 0 & 0 \\ P_{\gamma}^{T} H P_{\alpha} \circ U_{\alpha\gamma}^{T} & 0 & 0 \end{bmatrix} P^{T}$$

for all $H \in \mathcal{S}^n$. Then W is an element in $\partial_B \Pi_{\mathcal{S}^n_+}(A)$.

Let us come back to the IEQP. Denote

$$M =: \begin{bmatrix} M_1 & M_2 \\ M_2^T & M_4 \end{bmatrix}, \ C := \begin{bmatrix} C_1 & C_2 \\ C_2^T & C_4 \end{bmatrix},$$
$$K := \begin{bmatrix} K_1 & K_2 \\ K_2^T & K_4 \end{bmatrix},$$

where $M_1, C_1, K_1 \in S^k, M_2, C_2, K_2 \in \mathbb{R}^{k \times (n-k)}$, and $M_4, C_4, K_4 \in S^{(n-k)}$. Let $S := R\Lambda R^{-1}$.

For $(M, C, K) \in \Omega_0$, let $\mathcal{H}(M, C, K)$ be given by

$$\frac{1}{\sqrt{c_1}} (\Lambda^2)^T \left(R^T M_1 R \right) + \frac{1}{\sqrt{c_2}} \Lambda^T \left(R^T C_1 R \right) + \left(R^T K_1 R \right)$$

and $\mathcal{G}(M, C, K)$ be given by

$$\frac{1}{\sqrt{c_1}} (S^2)^T M_2 + \frac{1}{\sqrt{c_2}} S^T C_2 + K_2.$$

While $\mathcal{G}: \Omega_0 \to \mathbb{R}^{k \times (n-k)}$ is onto, $\mathcal{H}: \Omega_0 \to \mathbb{R}^{k \times k}$ is not. Let

 $\operatorname{Range}(\mathcal{H}) := \{\mathcal{H}(M, C, K) : (M, C, K) \in \Omega_0\}.$

 $\mathcal{H}: \Omega_0 \to \operatorname{Range}(\mathcal{H})$ is surjective. The dimension of $\operatorname{Range}(\mathcal{H})$ is given by

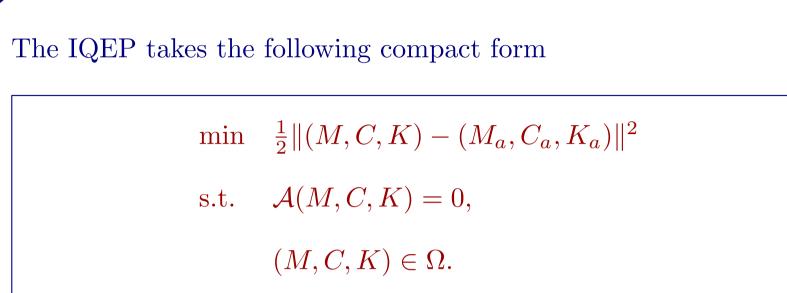
$$k^{2} - \sum_{i=1}^{\mu} s_{i}(s_{i}-1) - \frac{1}{2} \sum_{i=\mu+1}^{\nu} s_{i}(s_{i}-1).$$

In particular, if $s_1 = \cdots = s_{\mu} = s_{\mu+1} = \cdots = s_{\nu} = 1$, it is equal to k^2 .

Define the linear operator $\mathcal{A}: \Omega_0 \to \operatorname{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$ by

 $\mathcal{A}(M,C,K) := (\mathcal{H}(M,C,K), \mathcal{G}(M,C,K)).$

(1)



Define θ : Range $(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)} \to \mathbb{R}$ by

$$\theta(Y,Z): = \frac{1}{2} \|\Pi_{\Omega}((M_a, C_a, K_a) + \mathcal{A}^*(Y,Z))\|^2 -\frac{1}{2} \|(M_a, C_a, K_a)\|^2,$$

where $(Y, Z) \in \text{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$.

(2)

The dual problem is

min
$$\theta(Y, Z)$$

s.t. $(Y, Z) \in \text{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$.

Define $F : \operatorname{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)} \to \operatorname{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$ by

$$F(Y,Z) := \nabla \theta(Y,Z)$$

$$= \mathcal{A} \Pi_{\Omega} \left((M_a, C_a, K_a) + \mathcal{A}^*(Y,Z) \right),$$
(3)

where $(Y, Z) \in \text{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$.

(Newton's Method)

[Step 0.] Given $(Y^0, Z^0) \in \text{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}, \eta \in (0, 1),$ $\rho, \delta \in (0, 1/2). \ j := 0.$

[Step 1.] Select an element

$$W_j \in \partial \Pi_{\Omega} \left((M_a, C_a, K_a) + \mathcal{A}^*(Y^j, Z^j) \right)$$

and let

 $V_j := \mathcal{A} W_j \mathcal{A}^*.$

Apply the conjugate gradient method to find an approximate solution

$$(\Delta Y^j, \Delta Z^j) \in \operatorname{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}$$

to the linear system

$$F(Y^j, Z^j) + V_j(\Delta Y, \Delta Z) = 0$$
(4)

such that

$$\|F(Y^{j}, Z^{j}) + V_{j}(\Delta Y^{j}, \Delta Z^{j})\| \le \eta_{j} \|F(Y^{j}, Z^{j})\|$$
(5)

and

$$\left\langle F(Y^{j}, Z^{j}), (\Delta Y^{j}, \Delta Z^{j}) \right\rangle$$

$$\leq -\eta_{j} \left\langle (\Delta Y^{j}, \Delta Z^{j}), (\Delta Y^{j}, \Delta Z^{j}) \right\rangle,$$

$$(6)$$

where $\eta_j := \min\{\eta, \|F(Y^j, Z^j)\|\}.$

If (5) and (6) are not achievable, let

$$(\Delta Y^j, \Delta Z^j) := -F(Y^j, Z^j)$$
$$= -\mathcal{A} \prod_{\Omega} \left((M_a, C_a, K_a) + \mathcal{A}^*(Y^j, Z^j) \right).$$

[Step 2.] Let m_j be the smallest nonnegative integer m such that

$$\theta\left((Y^{j}, Z^{j}) + \rho^{m}(\Delta Y^{j}, \Delta Z^{j})\right) - \theta(Y^{j}, Z^{j})$$

$$\leq \delta\rho^{m}\left\langle F(Y^{j}, Z^{j}), (\Delta Y^{j}, \Delta Z^{j})\right\rangle.$$

Set

$$(Y^{j+1}, Z^{j+1}) := (Y^j, Z^j) + \rho^{m_j}(\Delta Y^j, \Delta Z^j).$$

[Step 3.] Replace j by j + 1 and go to Step 1.

Theorem 2. The algorithm generates an infinite sequence $\{(Y^j, Z^j)\}$ with the properties that for each $j \ge 0$, $(Y^j, Z^j) \in \text{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)}, \{(Y^j, Z^j)\}$ is bounded, and any accumulation point of $\{(Y^j, Z^j)\}$ is a solution to the dual problem.

For discussions on the rate of convergence, we need the constraint nondegenerate condition ("LICQ")

$$\mathcal{A}\left(\ln\left(\mathcal{T}_{\mathcal{S}^{n}_{+}}(\overline{M})\right), \mathcal{S}^{n}, \ln\left(\mathcal{T}_{\mathcal{S}^{n}_{+}}(\overline{K})\right)\right)$$
$$= \operatorname{Range}(\mathcal{H}) \times \mathbb{R}^{k \times (n-k)},$$

where $(\overline{M}, \overline{C}, \overline{K}) \in \Omega_0$ is a feasible solution to the original problem.

Theorem 3. Let $(\overline{Y}, \overline{Z})$ be an accumulation point of the infinite sequence $\{(Y^j, Z^j)\}$ generated by the algorithm. Let

$$(\overline{M},\overline{C},\overline{K}) := \Pi_{\Omega} \left((M_a, C_a, K_a) + \mathcal{A}^*(\overline{Y},\overline{Z}) \right).$$

Assume that the constraint nondegenerate condition holds at $(\overline{M}, \overline{C}, \overline{K})$. Then the whole sequence $\{(Y^j, Z^j)\}$ converges to $(\overline{Y}, \overline{Z})$ quadratically.

The stopping criterion is

$$\operatorname{Tol.} := \frac{\|\nabla \theta(Y_k, Z_k)\|}{\max\left\{1, \left\|\left(\frac{1}{\sqrt{c_1}}M_a, \frac{1}{\sqrt{c_2}}C_a, K_a\right)\right\|\right\}} \le 10^{-7}.$$

We set other parameters used in our algorithm as $\eta = 10^{-6}$, $\rho = 0.5$, and $\delta = 10^{-4}$.

$k = 30, c_1 = c_2 = 1.0$							
n	cputime	It.	Func.	Tol.			
100	$01~\mathrm{m}~26~\mathrm{s}$	18	24	3.9×10^{-11}			
200	04 m 39 s	14	15	3.9×10^{-11}			
500	$21~\mathrm{m}~16~\mathrm{s}$	11	12	1.3×10^{-10}			
1,000	$44~\mathrm{m}~13~\mathrm{s}$	9	10	1.1×10^{-9}			
1,500	08 h 49 m 11 s	7	8	$1.6 imes 10^{-8}$			
2,000	05 h 24 m 37 s	9	10	3.3×10^{-8}			

$k \approx n/3, c_1 = 10.0, c_2 = 0.10$								
n	k	$\operatorname{cputime}$	It.	Func.	Tol.			
100	33	46.1 s	9	11	1.4×10^{-9}			
200	66	$42~\mathrm{m}~42~\mathrm{s}$	13	15	5.8×10^{-8}			
300	100	02 h 24 m 23 s	17	20	6.5×10^{-9}			
400	133	04 h 38 m 42 s	10	11	4.0×10^{-8}			
450	150	12 h 23 m 44 s	13	14	8.8×10^{-9}			

The largest numerical examples that we tested in this paper are: (i) n = 2,000 and k = 30 and (ii) n = 450 and k = 150.

For case (i), there are roughly 6,000,000 unknowns in the primal problem and 60,000 unknowns in the dual problem while for case (ii), these numbers are roughly 300,000 and 67,000, respectively. In consideration of the scales of problems solved, our algorithm is very effective.