Numerical Methods

for Inverse Eigenvalue Problems

by

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A Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in

Mathematics

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Abstract

Abstract of thesis entitled:

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Submitted by BAI Zheng Jian

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An inverse eigenvalue problem is to determine a structured matrix from a given spectral data. Inverse eigenvalue problems arise in many applications, including control design, system identification, seismic tomography, principal component analysis, exploration and remote sensing, antenna array processing, geophysics, molecular spectroscopy, particle physics, structure analysis, circuit theory, Hopfield neural networks, mechanical system simulation, and so on. There is a large literature on the theoretic and the algorithmic aspects of inverse eigenvalue problems. In this thesis, we first note that Method III, originally proposed by Friedland, Nocedal, and Overton [SIAM J. Numer. Anal., 24 (1987), pp. 634–667] for solving inverse eigenvalue problems, is a Newton-type method. When the inverse problem is large, one can solve the Jacobian equation by iterative methods. However, iterative methods usually oversolve the problem in the sense that they require far more (inner) iterations than is required for the convergence of the Newton (outer) iterations. To overcome the shortcoming of Method III, we provide an inexact method, called inexact Cayley transform method, for solving inverse eigenvalue problems. Our inexact Cayley transform method can minimize the oversolving problem and improve the efficiency. Then we consider the solvability of the inverse eigenproblems for two special classes of matrices. The sufficient and necessary conditions are obtained. Also, we discuss the best approximation problems for the two special inverse eigenproblems. We show that the best approximations are unique and provide explicit expressions for the optimal solution. Moreover, we respectively propose the algorithms for computing the optimal solutions to the two best approximation problems.

The thesis is composed of the following papers, which will be referred to in the text by the capital letters A–C.

- [A] Z. Bai, R. Chan, and B. Morini, An Inexact Cayley Transform Method for Inverse Eigenvalue Problems, submitted.
- [B] Z.J. Bai, The Solvability Conditions for the Inverse Eigenvalue Problem of Hermitian and Generalized Skew-Hamiltonian Matrices and Its Approximation, Inverse Problems, 19 (2003), 1185–1194.
- [C] Z.J. Bai and R.H. Chan, Inverse Eigenproblem for Centrosymmetric and Centroskew Matrices and Their Approximation, Theoret. Comput. Sci., 315 (2004), 309–318.

DECLARATION

The author declares that the thesis represents his own work based on the ideas suggested by Prof. Raymond H. Chan, the author's supervisor. All the work is done under the supervision of Prof. Raymond H. Chan during the period 2001–2004 for the degree of Doctor of Philosophy at The Chinese University of Hong Kong. The work submitted has not been previously included in a thesis, dissertation of report submitted to any institution of a degree, diploma or other qualifications.

BAI, Zheng Jian

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To

My Family

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1 Introduction

Let A_0, A_1, \ldots, A_n be real symmetric *n*-by-*n* matrices. For any vector $\mathbf{c} = (c_1, c_2, \ldots, c_n)^T \in \mathbb{R}^n$, we define the matrix $A(\mathbf{c})$ by

$$A(\mathbf{c}) \equiv A_0 + \sum_{i=1}^n c_i A_i.$$

We denote the eigenvalues of $A(\mathbf{c})$ by $\{\lambda_i(\mathbf{c})\}_{i=1}^n$ with $\lambda_1(\mathbf{c}) \leq \lambda_2(\mathbf{c}) \leq \cdots \leq \lambda_n(\mathbf{c})$. The inverse eigenvalue problem is defined as follows:

IEP: Given *n* real numbers $\lambda_1^* \leq \cdots \leq \lambda_n^*$, find a vector $\mathbf{c}^* \in \mathbb{R}^n$ such that

$$\lambda_i(\mathbf{c}^*) = \lambda_i^* \text{ for } i = 1, \dots, n.$$

In particular, there are two special cases of the IEP, i.e. the additive and multiplicative inverse eigenvalue problems. The IEP has been used successfully in a variety of applications. The classical example is the solution of inverse Sturm-Liouville problems, see for instance Borg [8], Gelfand and Levitan [30], Downing and Householder [22], Osborne [47] and Hald [34]. The IEP also appears in studying a vibrating string (see for instance Zhou and Dai [61]) and Downing and Householder [22]), nuclear spectroscopy (see for instance Brussard and Glaudemans [9]) and molecular spectroscopy (see for instance Pliva and Toman [48] and Friedland [28]). In addition, there are some variations of the IEP arising in factor analysis (see for instance Harman [35]) and the educational testing problem (see for instance Chu and Wright [18], Friedland [26] and Fletcher [24]). There is a rich literature on the theoretic and the numerical aspects of the IEP. By using the techniques from algebraic curves, degree theory, or algebraic geometry, there are some necessary and sufficient conditions on the solvability of the IEP. For some conditions on the existence and uniqueness of solutions to additive inverse eigenvalue problems, see, for examples, [1, 27, 10, 4, 32, 40, 41, 45, 49, 52, 53, 58, 59]. For the solvability to the multiplicative inverse eigenvalue problems, see for instance [21, 33, 46, 50, 54]. There are also many numerical algorithms developed for computational purposes. A partial list for solving the additive inverse eigenvalue problems, includes, for examples, [5, 6, 7, 22, 29, 34, 43, 44, 56].

The attempt to collect the inverse eigenvalue problems, to identify and classify their characteristics, and to summarize current developments in both the theoretic and the algorithmic aspects was made by many authors such as Zhou and Dai [61], Xu [58], Chu [14, 15] and Chu and Golub [16].

Four numerical methods for the IEP have been surveyed by Friedland, Nocedal, and Overton [29] for solving the general IEP. We first note that one of these methods, Method III, is a Newton-type method. When the inverse problem

is large, iterative methods are used to solve the Jacobian equation. However, iterative methods usually oversolve the problem in the sense that they require far more (inner) iterations than is required for the convergence of the Newton (outer) iterations. For minimizing the oversolving problem and improving the efficiency, we have to look for new approaches to reduce or minimize the oversolving problem and improve the efficiency. For solving the oversolving problem, based on Method II in [29], Chan, Chung, and Xu [11] have proposed an inexact Newton-like Method for the IEP when the problem is large. In this thesis, based on Method III in [29], we consider using the inexact Cayley transform method for solving the IEP when the problem is large. We give some practical experiments which illustrate our results.

We also consider the following two related problems:

Problem I: Given

$$X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m] \in \mathbb{C}^{n \times m}$$

and

$$\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_m) \in \mathbb{C}^{m \times m}$$

find a structured matrix $A \in \mathbb{C}^{n \times n}$ such that

$$AX = X\Lambda,$$

where $\mathbb{C}^{n \times m}$ denotes the set of all *n*-by-*m* complex matrices.

Problem II: Let \mathcal{L}_S be the solution set of Problem I. Given a matrix $\tilde{A} \in \mathbb{C}^{n \times n}$, find $A^* \in \mathcal{L}_S$ such that

$$\|\tilde{A} - A^*\| = \min_{A \in \mathcal{L}_S} \|\tilde{A} - A\|,$$

where $\|\cdot\|$ is the Frobenius norm.

The first problem initially appeared in the design of Hopfield neural networks [17, 42]. It is also applied to the design of vibration in mechanical, civil engineering and aviation [13]. The second problem occurs frequently in experimental design, see for instance [38, p.123]. Here the matrix \tilde{A} may be a matrix obtained from experiments, but it may not satisfy the structural requirement and/or spectral requirement. The best estimate A^* is the matrix that satisfies both restrictions and is the best approximation of \tilde{A} in the Frobenius norm, see for instance [2, 3, 36].

In this thesis, we discuss the two problems for two important special classes of matrices: Hermitian and generalized skew-Hamilton matrices and centrosymmetric matrices. For the two sets of structured matrices, we present the solvability conditions and provide the general solution formula for Problem I. Also we show the existence and uniqueness of the solution for Problem II, and then derive the expression of the solution when the solution set \mathcal{L}_S is nonempty, and finally we propose the algorithms to compute the solution to Problem II. We also give some illustrative numerical examples.

2 Summary of Papers A–C

In this section, we summarize the papers A–C and briefly review the main results.

2.1 Paper A

When the given eigenvalues are distinct, the IEP can be formulated as a nonlinear system of equations

$$\mathbf{f}(\mathbf{c}) = (\lambda_1(\mathbf{c}) - \lambda_1^*, \cdots, \lambda_n(\mathbf{c}) - \lambda_n^*)^T = \mathbf{0}.$$
 (1)

Four Newton-type methods for solving (1) were given by Friedland, Nocedal, and Overton [29]. When the IEP is large, Method III has an obvious disadvantage: the inversions will be costly. The cost can be reduced by using iterative methods (the inner iterations). Although an iterative method can reduce the complexity, it may *oversolve* the approximate Jacobian equation in the sense that the last tens or hundreds inner iterations before convergence may not improve the convergence of the outer Newton iterations [23]. The inexact Newton method stops the inner iterations before convergence. By choosing suitable stopping criteria, we can reduce the total cost of the whole inner-outer iterations.

In this paper, we consider an inexact Cayley transform method for solving the IEP. For general nonlinear equation $\mathbf{h}(\mathbf{c}) = \mathbf{0}$, the stopping criterion of inexact Newton methods is usually given in terms of $\mathbf{h}(\mathbf{c})$, see for instance [23, 25]. By (1), this will involve computing the exact eigenvalues $\lambda_i(\mathbf{c}^k)$ of $A(\mathbf{c}^k)$ which are costly to compute. Our idea is to replace them by the Rayleigh quotients. We

show that our inexact method converges superlinearly in the root sense and a good tradeoff between the required inner and outer iterations can be obtained. We can also observe the facts from our numerical tests.

2.2 Paper B

Hamiltonian and skew-Hamiltonian matrices play an important role in engineering, such as in linear-quadratic optimal control [37, 51], H_{∞} optimization [60], and the related problem of solving algebraic Riccati equations [39]. In this paper, we study Problems I and II related to Hermitian and generalized skew-Hamiltonian matrices.

2.3 Paper C

The centrosymmetric and centroskew matrices play an important role in many areas [19, 55] such as signal processing [20, 31], the numerical solution of differential equations [12], and Markov processes [57]. In this paper, we consider Problems I and II related to centrosymmetric and centroskew matrices.

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An Inexact Cayley Transform Method For Inverse Eigenvalue Problems

Abstract

The Cayley transform method is a Newton-like method for solving inverse eigenvalue problems. If the problem is large, one can solve the Jacobian equation by iterative methods. However, iterative methods usually oversolve the problem in the sense that they require far more (inner) iterations than is required for the convergence of the Newton (outer) iterations. In this paper, we develop an inexact version of the Cayley transform method. Our method can reduce the oversolving problem and improves the efficiency with respect to the exact version. We show that the convergence rate of our method is superlinear and that a good tradeoff between the required inner and outer iterations can be obtained.

1 Introduction

Inverse eigenvalue problems arise in a variety of applications, see for instances the pole assignment problem [3, 28], the inverse Toeplitz eigenvalue problem [6, 27, 31], the inverse Sturm-Liouville problem [1, 18], and also problems in applied mechanics and structure design [15, 16, 19], applied geophysics [26], applied physics [20], numerical analysis [23], and dynamics systems [11]. A good reference for these applications is the recent survey paper on structured inverse eigenvalue problems by Chu and Golub [8]. In many of these applications, the problem size n can be large. For example in the discrete inverse Sturm-Liouville problem, n is the number of grid-points, see Chu and Golub [8, p. 10]. Our goal in this paper is to derive an efficient algorithm for solving inverse eigenvalue problems when nis large.

Let us first define the notations. Let $\{A_k\}_{k=0}^n$ be n+1 real symmetric *n*-by-*n* matrices. For any $\mathbf{c} = (c_1, \ldots, c_n)^T \in \mathbb{R}^n$, let

$$A(\mathbf{c}) \equiv A_0 + \sum_{i=1}^n c_i A_i,\tag{1}$$

and denote the eigenvalues of $A(\mathbf{c})$ by $\{\lambda_i(\mathbf{c})\}_{i=1}^n$, where $\lambda_1(\mathbf{c}) \leq \lambda_2(\mathbf{c}) \leq \cdots \leq \lambda_n(\mathbf{c})$. An inverse eigenvalue problem (IEP) is defined as follows: Given *n* real numbers $\lambda_1^* \leq \cdots \leq \lambda_n^*$, find $\mathbf{c} \in \mathbb{R}^n$ such that $\lambda_i(\mathbf{c}) = \lambda_i^*$ for $i = 1, \ldots, n$.

We note that the IEP can be formulated as a system of nonlinear equations

$$\mathbf{f}(\mathbf{c}) \equiv (\lambda_1(\mathbf{c}) - \lambda_1^*, \dots, \lambda_n(\mathbf{c}) - \lambda_n^*)^T = \mathbf{0}.$$
 (2)

It is easy to see that a direct application of Newton method to (2) requires the computation of $\lambda_i(\mathbf{c})$ at each iteration. To overcome the drawback, different Newton-like methods for solving (2) are given in [14]. One of these methods, Method III, forms an approximate Jacobian equation by applying matrix exponentials and Cayley transforms. As noted in [5], the method is particularly interesting and it has been used or cited in [6, 7, 21, 29] for instances.

If (2) is solved by Newton-like methods, then in each Newton iteration (the outer iteration), we need to solve the approximate Jacobian equation. When n is large, solving such a linear system will be costly. The cost can be reduced by using iterative methods (the inner iterations). Although iterative methods can reduce the complexity, they may oversolve the approximate Jacobian equation in the sense that the last tens or hundreds inner iterations before convergence may not improve the convergence of the outer Newton iterations [10]. In order to alleviate the oversolving problem, we propose in this paper an inexact Newton-like method for solving the nonlinear system (2). The inexact Newton-like method is a method that stops the inner iterations before convergence. By choosing suitable stopping criteria, we can minimize the oversolving problem and therefore reduce the total cost of the whole inner-outer iterations. In essence, one does not need to solve the approximate Jacobian equation exactly in order that the Newton method converges fast.

In this paper, we give an inexact version of Method III where the approximate Jacobian equation is solved inexactly by stopping the inner iterations before convergence. We propose a new criterion to stop the inner iterations at each Newton step and provide theoretical and experimental results for the procedure. First, we will show that the convergence rate of our method is superlinear. Then, we illustrate by numerical examples that it can avoid the oversolving problem and thereby reduce the total cost of the inner-outer iterations.

We remark that our proposed method is locally convergent. Thus, how to

select the initial guess becomes a crucial problem. However, global continuous methods such as the homotopy method can be used in conjunction with our procedure. In these continuous methods, our inexact method can be used as the corrector step where a valid starting point is provided by the globalization strategy, see for examples [2] and [33, pp. 256–262].

This paper is organized as follows. In §2, we recall Method III for solving the IEP. In §3, we introduce our inexact method. In §4, we give the convergence analysis of our method. In §5, we present numerical tests to illustrate our results. In §6, we give some remarks on the case when multiple eigenvalues are present.

2 The Cayley Transform Method

Method III in [14] is based on Cayley transforms. In this section, we briefly recall this method. Let \mathbf{c}^* be a solution to the IEP. Then there exists an orthogonal matrix Q_* satisfying

$$Q_*^T A(\mathbf{c}^*) Q_* = \Lambda_*, \quad \Lambda_* = \operatorname{diag}(\lambda_1^*, \dots, \lambda_n^*).$$
(3)

Suppose that \mathbf{c}^k and Q_k are the current approximations of \mathbf{c}^* and Q_* in (3) respectively and that Q_k is an orthogonal matrix. Define $e^{Z_k} \equiv Q_k^T Q_*$. Then Z_k is a skew-symmetric matrix and (3) can be written as

$$Q_k^T A(\mathbf{c}^*) Q_k = e^{Z_k} \Lambda_* e^{-Z_k} = (I + Z_k + \frac{1}{2} (Z_k)^2 + \dots) \Lambda_* (I - Z_k + \frac{1}{2} (Z_k)^2 + \dots).$$

Thus $Q_k^T A(\mathbf{c}^*) Q_k = \Lambda_* + Z_k \Lambda_* - \Lambda_* Z_k + O(||Z_k||^2)$, where $||\cdot||$ denotes the 2-norm.

In Method III, \mathbf{c}^k is updated by neglecting the second order terms in Z_k , i.e.

$$Q_k^T A(\mathbf{c}^{k+1}) Q_k = \Lambda_* + Z_k \Lambda_* - \Lambda_* Z_k.$$
(4)

We find \mathbf{c}^{k+1} by equating the diagonal elements in (4), i.e. \mathbf{c}^{k+1} is given by

$$(\mathbf{q}_i^k)^T A(\mathbf{c}^{k+1}) \mathbf{q}_i^k = \lambda_i^*, \quad i = 1, \dots, n,$$
(5)

where $\{\mathbf{q}_{i}^{k}\}_{i=1}^{n}$ are the column vectors of Q_{k} . By (1), (5) can be rewritten as a linear system

$$J^{(k)}\mathbf{c}^{k+1} = \boldsymbol{\lambda}^* - \mathbf{b}^{(k)},\tag{6}$$

where $\boldsymbol{\lambda}^* \equiv (\lambda_1^*, \dots, \lambda_n^*)^T$, and

$$\left[J^{(k)}\right]_{ij} = (\mathbf{q}_i^k)^T A_j \mathbf{q}_i^k, \quad i, j = 1, \dots, n,$$
(7)

$$[\mathbf{b}^{(k)}]_i = (\mathbf{q}_i^k)^T A_0 \mathbf{q}_i^k, \quad i = 1, \dots, n.$$
(8)

Once we get \mathbf{c}^{k+1} from (6), we obtain Z_k by equating the off-diagonal elements in (4), i.e.

$$[Z_k]_{ij} = \frac{(\mathbf{q}_i^k)^T A(\mathbf{c}^{k+1}) \mathbf{q}_j^k}{\lambda_j^* - \lambda_i^*}, \qquad 1 \le i \ne j \le n.$$
(9)

Finally we update Q_k by setting $Q_{k+1} = Q_k U_k$, where U_k is an orthogonal matrix constructed by the Cayley transform for e^{Z_k} , i.e.

$$U_k = (I + \frac{1}{2}Z_k)(I - \frac{1}{2}Z_k)^{-1}.$$

We summarize the algorithm here.

Algorithm I: Cayley Transform Method

- 1. Given \mathbf{c}^0 , compute the orthonormal eigenvectors $\{\mathbf{q}_i(\mathbf{c}^0)\}_{i=1}^n$ of $A(\mathbf{c}^0)$. Let $Q_0 = [\mathbf{q}_1^0, \dots, \mathbf{q}_n^0] = [\mathbf{q}_1(\mathbf{c}^0), \dots, \mathbf{q}_n(\mathbf{c}^0)].$
- 2. For $k = 0, 1, 2, \ldots$, until convergence, do:
 - (a) Form the approximate Jacobian matrix $J^{(k)}$ by (7) and $\mathbf{b}^{(k)}$ by (8).
 - (b) Solve \mathbf{c}^{k+1} from the approximate Jacobian equation (6).
 - (c) Form the skew-symmetric matrix Z_k by (9).
 - (d) Compute $Q_{k+1} = [\mathbf{q}_1^{k+1}, \dots, \mathbf{q}_n^{k+1}] = [\mathbf{w}_1^{k+1}, \dots, \mathbf{w}_n^{k+1}]^T$ by solving $(I + \frac{1}{2}Z_k)\mathbf{w}_j^{k+1} = \mathbf{g}_j^k, \quad j = 1, \cdots, n,$ (10)

where \mathbf{g}_{j}^{k} is the *j*th column of $G_{k} = (I - \frac{1}{2}Z_{k})Q_{k}^{T}$.

This method was proved to converge quadratically in [14]. Note that in each outer iteration (i.e. Step 2), we have to solve the linear systems (6) and (10). When the systems are large, we may reduce the computational cost by solving both systems iteratively. One could expect that it requires only a few iterations to solve (10) iteratively. This is due to the fact that, as $\{\mathbf{c}^k\}$ converges to \mathbf{c}^* , $\|Z_k\|$ converges to zero, see [14, Equation (3.64)]. Consequently, the coefficient matrix on the left hand side of (10) approaches the identity matrix in the limit, and therefore (10) can be solved efficiently by iterative methods. On the other hand, iterative methods may oversolve the approximate Jacobian equation (6), in the sense that for each outer Newton iteration, the last few inner iterations may not contribute much to the convergence of the outer iterations. How to stop the inner iterations efficiently is the focus of our next section.

3 The Inexact Cayley Transform Method

The main aim of this paper is to propose an efficient version of Algorithm I for large problems. To reduce the computational cost, we solve both (6) and (10) iteratively with (6) being solved inexactly. First, we derive a computable stopping criterion for (6), then we establish the convergence rate of the resulting procedure.

For general nonlinear equation $\mathbf{f}(\mathbf{c}) = \mathbf{0}$, the stopping criterion of inexact Newton methods is usually given in terms of $\mathbf{f}(\mathbf{c})$, see for instances [10, 12, 22]. By (2), this will involve computing $\lambda_i(\mathbf{c}^k)$ of $A(\mathbf{c}^k)$ which are costly to compute. Our idea is to replace them by the Rayleigh quotients, see (14) and (16) below. We will prove in §4 that this replacement will retain superlinear convergence.

Algorithm II: Inexact Cayley Transform Method

1. Given \mathbf{c}^0 , compute the orthonormal eigenvectors $\{\mathbf{q}_i(\mathbf{c}^0)\}_{i=1}^n$ and the eigenvalues $\{\lambda_i(\mathbf{c}^0)\}_{i=1}^n$ of $A(\mathbf{c}^0)$. Let $P_0 = [\mathbf{p}_1^0, \dots, \mathbf{p}_n^0] = [\mathbf{q}_1(\mathbf{c}^0), \dots, \mathbf{q}_n(\mathbf{c}^0)]$, and

$$\boldsymbol{\rho}^0 = (\lambda_1(\mathbf{c}^0), \ldots, \lambda_n(\mathbf{c}^0))^T.$$

- 2. For $k = 0, 1, 2, \ldots$, until convergence, do:
 - (a) Form the approximate Jacobian matrix J_k and \mathbf{b}^k as follows:

$$[J_k]_{ij} = (\mathbf{p}_i^k)^T A_j \mathbf{p}_i^k, \quad 1 \le i, j \le n,$$
(11)

$$[\mathbf{b}^k]_i = (\mathbf{p}_i^k)^T A_0 \mathbf{p}_i^k, \quad 1 \le i \le n.$$
(12)

(b) Solve \mathbf{c}^{k+1} inexactly from the approximate Jacobian equation:

$$J_k \mathbf{c}^{k+1} = \boldsymbol{\lambda}^* - \mathbf{b}^k + \mathbf{r}^k, \tag{13}$$

until the residual \mathbf{r}^k satisfies

$$\|\mathbf{r}^{k}\| \leq \frac{\|\boldsymbol{\rho}^{k} - \boldsymbol{\lambda}^{*}\|^{\beta}}{\|\boldsymbol{\lambda}^{*}\|^{\beta}}, \quad \beta \in (1, 2].$$
(14)

(c) Form the skew-symmetric matrix Y_k :

$$[Y_k]_{ij} = \frac{(\mathbf{p}_i^k)^T A(\mathbf{c}^{k+1}) \mathbf{p}_j^k}{\lambda_j^* - \lambda_i^*}, \quad 1 \le i \ne j \le n$$

(d) Compute $P_{k+1} = [\mathbf{p}_1^{k+1}, \dots, \mathbf{p}_n^{k+1}] = [\mathbf{v}_1^{k+1}, \dots, \mathbf{v}_n^{k+1}]^T$ by solving $(I + \frac{1}{2}Y_k)\mathbf{v}_j^{k+1} = \mathbf{h}_j^k, \quad j = 1, \cdots, n,$ (15)

where \mathbf{h}_{j}^{k} is the *j*th column of $H_{k} = (I - \frac{1}{2}Y_{k})P_{k}^{T}$.

(e) Compute $\boldsymbol{\rho}^{k+1} = (\rho_1^{k+1}, \dots, \rho_n^{k+1})^T$ by $\rho_i^{k+1} = (\mathbf{p}_i^{k+1})^T A(\mathbf{c}^{k+1}) \mathbf{p}_i^{k+1}, \quad i = 1, \dots, n.$ (16)

Since P_0 is an orthogonal matrix and Y_k are skew-symmetric matrices, we see that P_k so generated by the Cayley transform in (15) must be orthogonal, i.e.

$$P_k^T P_k = I, \quad k = 0, 1, \dots$$
 (17)

To maintain the orthogonality of P_k , that would mean that (15) cannot be solved inexactly. However, we will see in §4 that $||Y_k||$ converges to zero as \mathbf{c}^k converges to \mathbf{c}^* (see (35) and (44)). Consequently, the matrix on the left hand side of (15) approaches the identity matrix in the limit. Therefore we can expect to solve (15) accurately by iterative methods using just a few iterations.

The expensive step in Algorithm II will be the solution of (13). The aim of our next section is to show that with our stopping criterion in (14), the convergence rate of Algorithm II is equal to β given in (14).

4 Convergence Analysis

In the following, we let \mathbf{c}^k be the *k*th iterate produced by Algorithm II, and $\{\lambda_i(\mathbf{c}^k)\}_{i=1}^n$ and $\{\mathbf{q}_i(\mathbf{c}^k)\}_{i=1}^n$ be the eigenvalues and normalized eigenvectors of $A(\mathbf{c}^k)$. We let $Q_* = [\mathbf{q}_1(\mathbf{c}^*), \dots, \mathbf{q}_n(\mathbf{c}^*)]$ be the orthogonal matrix of the eigenvectors of $A(\mathbf{c}^*)$. Moreover, we define

$$E_k \equiv P_k - Q_*,\tag{18}$$

the error matrix at the kth outer iteration. As in [14], we assume that the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ are distinct and that the Jacobian $J(\mathbf{c}^*)$ defined by

$$\left[J(\mathbf{c}^*)\right]_{ij} \equiv \mathbf{q}_i(\mathbf{c}^*)^T A_j \mathbf{q}_i(\mathbf{c}^*), \quad 1 \le i, j \le n,$$
(19)

is nonsingular.

4.1 Preliminary Lemmas

In this subsection, we prove some preliminary results which are necessary for the convergence analysis of our method. First we list three lemmas that are already proven in other papers.

Lemma 1 Let the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ be distinct and $\mathbf{q}_i(\mathbf{c}^*)$ be the normalized eigenvectors of $A(\mathbf{c}^*)$ corresponding to λ_i^* for i = 1, ..., n. Then there exist positive numbers δ_0 and τ_0 such that, if $\|\mathbf{c}^k - \mathbf{c}^*\| \leq \delta_0$, we get

$$\|\mathbf{q}_i(\mathbf{c}^k) - \mathbf{q}_i(\mathbf{c}^*)\| \le \tau_0 \|\mathbf{c}^k - \mathbf{c}^*\|, \quad 1 \le i \le n.$$

$$(20)$$

Proof: It follows from the analyticity of eigenvectors corresponding to simple eigenvalues, see for instances [33, p. 249, Equation (4.6.13)].

Lemma 2 Let J_k , $J(\mathbf{c}^*)$ and E_k be defined as in (11), (19) and (18) respectively. Then $||J_k - J(\mathbf{c}^*)|| = O(||E_k||)$. Hence if $J(\mathbf{c}^*)$ is nonsingular, then there exist positive numbers ϵ_0 and τ_1 such that if $||E_k|| \leq \epsilon_0$, then J_k is nonsingular and

$$\|J_k^{-1}\| \le \tau_1. \tag{21}$$

Proof: The first part follows easily from the formula of J_k and $J(\mathbf{c}^*)$, and the second part follows from the continuity of matrix inverses, cf. [4] or [33, p. 249, Equation (4.6.11)].

Lemma 3 [14, Corollary 3.1] There exist two positive numbers ϵ_1 and τ_2 such that, if $||E_k|| \leq \epsilon_1$, the skew-symmetric matrix X_k defined by $e^{X_k} \equiv P_k^T Q_*$ satisfies $||X_k|| \leq \tau_2 ||E_k||$.

We now express our stopping criteria (14) in terms of $\|\mathbf{c}^k - \mathbf{c}^*\|$ and $\|E_k\|$.

Lemma 4 Let the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ be distinct and $\boldsymbol{\rho}^k$ be given by (16). Then for $k \ge 0$,

$$\|\boldsymbol{\rho}^{k} - \boldsymbol{\lambda}^{*}\| = O(\|\mathbf{c}^{k} - \mathbf{c}^{*}\| + \|E_{k}\|).$$
(22)

Proof: By (16), $\rho_i^k = (\mathbf{p}_i^k)^T A(\mathbf{c}^k) \mathbf{p}_i^k$. For $1 \le i \le n$, we write

$$|\rho_i^k - \lambda_i^*| \le |(\mathbf{p}_i^k)^T A(\mathbf{c}^k) \mathbf{p}_i^k - (\mathbf{p}_i^k)^T A(\mathbf{c}^*) \mathbf{p}_i^k| + |(\mathbf{p}_i^k)^T A(\mathbf{c}^*) \mathbf{p}_i^k - \lambda_i^*|.$$
(23)

We claim that each term in the right hand side of (23) is bounded by $O(||\mathbf{c}^k - \mathbf{c}^*|| + ||E_k||)$. For the first term, by (1) and (17), we have

$$|(\mathbf{p}_{i}^{k})^{T}A(\mathbf{c}^{k})\mathbf{p}_{i}^{k} - (\mathbf{p}_{i}^{k})^{T}A(\mathbf{c}^{*})\mathbf{p}_{i}^{k}| = |(\mathbf{p}_{i}^{k})^{T}\sum_{j=1}^{n}(c_{j}^{k} - c_{j}^{*})A_{j}\mathbf{p}_{i}^{k}| = O(||\mathbf{c}^{k} - \mathbf{c}^{*}||).$$
(24)

For the second term, we have

$$\begin{aligned} |(\mathbf{p}_{i}^{k})^{T} A(\mathbf{c}^{*}) \mathbf{p}_{i}^{k} - \lambda_{i}^{*}| \\ &= |(\mathbf{p}_{i}^{k})^{T} A(\mathbf{c}^{*}) \mathbf{p}_{i}^{k} - (\mathbf{q}_{i}(\mathbf{c}^{*}))^{T} A(\mathbf{c}^{*}) \mathbf{q}_{i}(\mathbf{c}^{*})| \\ &\leq |(\mathbf{p}_{i}^{k})^{T} A(\mathbf{c}^{*}) \mathbf{p}_{i}^{k} - (\mathbf{q}_{i}(\mathbf{c}^{*}))^{T} A(\mathbf{c}^{*}) \mathbf{p}_{i}^{k}| \\ &+ |(\mathbf{q}_{i}(\mathbf{c}^{*}))^{T} A(\mathbf{c}^{*}) \mathbf{p}_{i}^{k} - (\mathbf{q}_{i}(\mathbf{c}^{*}))^{T} A(\mathbf{c}^{*}) \mathbf{q}_{i}(\mathbf{c}^{*})| \\ &\leq (||\mathbf{p}_{i}^{k}|| + ||\mathbf{q}_{i}(\mathbf{c}^{*})||) ||A(\mathbf{c}^{*})|| ||\mathbf{q}_{i}(\mathbf{c}^{*}) - \mathbf{p}_{i}^{k}|| \leq O(||\mathbf{p}_{i}^{k} - \mathbf{q}_{i}(\mathbf{c}^{*})||). \end{aligned}$$

Since $[\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)]$ is the *i*th column of E_k , $\|\mathbf{p}_i^k - \mathbf{q}_i(\mathbf{c}^*)\| \le \|E_k\|$, and we have

$$|(\mathbf{p}_i^k)^T A(\mathbf{c}^*) \mathbf{p}_i^k - \lambda_i^*| = O(||E_k||), \quad 1 \le i \le n.$$
(25)

Putting (24) and (25) into (23), we have (22).

As remarked already, the main difference between Algorithm II and Algorithm I is that we solve (13) approximately rather than exactly as in (6). Thus by comparing with (4), we see that the matrix Y_k and vector \mathbf{c}^{k+1} of Algorithm II are defined by

$$\Lambda_* + Y_k \Lambda_* - \Lambda_* Y_k = P_k^T A(\mathbf{c}^{k+1}) P_k - R_k, \qquad (26)$$

where $R_k = \text{diag}([\mathbf{r}^k]_1, \dots, [\mathbf{r}^k]_n)$ and $[\mathbf{r}^k]_i$ is the *i*th entry of the residual vector \mathbf{r}^k given in (13). Using (26), we can estimate $\|\mathbf{c}^{k+1} - \mathbf{c}^*\|$ and $\|E_{k+1}\|$ in terms of $\|\mathbf{c}^k - \mathbf{c}^*\|$ and $\|E_k\|$.

Lemma 5 Let the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ be distinct and the Jacobian $J(\mathbf{c}^*)$ defined in (19) be nonsingular. Then there exist two positive numbers δ_1 and ϵ_2

such that the conditions $\|\mathbf{c}^k - \mathbf{c}^*\| \leq \delta_1$ and $\|E_k\| \leq \epsilon_2$ imply

$$\|\mathbf{c}^{k+1} - \mathbf{c}^*\| = O(\|\boldsymbol{\rho}^k - \boldsymbol{\lambda}^*\|^\beta + \|E_k\|^2), \qquad (27)$$

$$||E_{k+1}|| = O(||\mathbf{c}^{k+1} - \mathbf{c}^*|| + ||E_k||^2).$$
(28)

Proof: Let X_k be defined by $e^{X_k} \equiv P_k^T Q_*$. By Lemma 3, if $||E_k|| \leq \epsilon_1$, then

$$||X_k|| = O(||E_k||).$$
(29)

By (3), $e^{X_k} \Lambda_* e^{-X_k} = P_k^T A(\mathbf{c}^*) P_k$. Hence, if $||E_k||$ is small enough, we have

$$\Lambda_* + X_k \Lambda_* - \Lambda_* X_k = P_k^T A(\mathbf{c}^*) P_k + O(||E_k||^2).$$
(30)

Subtracting (26) from (30), we have

$$(X_k - Y_k)\Lambda_* - \Lambda_*(X_k - Y_k) = P_k^T(A(\mathbf{c}^*) - A(\mathbf{c}^{k+1}))P_k + R_k + O(||E_k||^2).$$
(31)

Equating the diagonal elements yields

$$J_k(\mathbf{c}^{k+1} - \mathbf{c}^*) = \mathbf{r}^k + O(||E_k||^2),$$

where J_k is defined by (11). Thus if $||E_k||$ is sufficiently small, then by (21) and (14), we get (27).

To get (28), we note from (15) that

$$E_{k+1} = P_{k+1} - Q^*$$

= $P_k \left[(I + \frac{1}{2}Y_k) (I - \frac{1}{2}Y_k)^{-1} - e^{X_k} \right]$
= $P_k \left[(I + \frac{1}{2}Y_k) - (I + X_k + O(||X_k||^2)) (I - \frac{1}{2}Y_k) \right] (I - \frac{1}{2}Y_k)^{-1}$
= $P_k \left[Y_k - X_k + O(X_kY_k + ||X_k||^2) \right] (I - \frac{1}{2}Y_k)^{-1}.$

Therefore by (17) and (29), we have

$$||E_{k+1}|| \le \left[||Y_k - X_k|| + O(||E_k|| ||Y_k|| + ||E_k||^2) \right] ||(I - \frac{1}{2}Y_k)^{-1}||.$$
(32)

We now estimate the norms in the right hand side of (32) one by one. For $1 \le i \ne j \le n$, the off-diagonal equations of (31) give

$$[X_k]_{ij} - [Y_k]_{ij} = \frac{1}{\lambda_j^* - \lambda_i^*} (\mathbf{p}_i^k)^T (A(\mathbf{c}^*) - A(\mathbf{c}^{k+1})) \mathbf{p}_j^k + O(||E_k||^2).$$

It follows that

$$|[X_k]_{ij} - [Y_k]_{ij}| = O(||\mathbf{c}^{k+1} - \mathbf{c}^*|| + ||E_k||^2),$$

and hence

$$||X_k - Y_k|| \leq ||X_k - Y_k||_F = O(||\mathbf{c}^{k+1} - \mathbf{c}^*|| + ||E_k||^2),$$
(33)

where $\|\cdot\|_F$ denotes the Frobenius norm. By (29) and (33),

$$||Y_k|| = O(||\mathbf{c}^{k+1} - \mathbf{c}^*|| + ||E_k|| + ||E_k||^2).$$
(34)

By (27) and (22), we have

$$||Y_k|| = O(||\boldsymbol{\rho}^k - \boldsymbol{\lambda}^*||^\beta + ||E_k||) = O((||\mathbf{c}^k - \mathbf{c}^*|| + ||E_k||)^\beta + ||E_k||).$$
(35)

Thus if $\|\mathbf{c}^k - \mathbf{c}^*\|$ and $\|E_k\|$ are sufficiently small, we have $\|Y_k\| \le 1$, and therefore

$$\|(I - \frac{1}{2}Y_k)^{-1}\| \le \frac{1}{1 - \frac{1}{2}}\|Y_k\| \le 2.$$
(36)

Finally, by putting (33), (34) and (36) into (32), we have (28). $\hfill \Box$

4.2 Convergence Rate of Algorithm II

In the following, we show that the root-convergence rate of our method is at least β . Here, we recall the definition of root-convergence, see [25, Chap. 9].

Definition 1 Let $\{\mathbf{x}^k\}$ be a sequence with limit \mathbf{x}^* . Then the numbers

$$R_p\{\mathbf{x}^k\} = \begin{cases} \limsup_{k \to \infty} \|\mathbf{x}^k - \mathbf{x}^*\|^{1/k}, & \text{if } p = 1, \\ \limsup_{k \to \infty} \|\mathbf{x}^k - \mathbf{x}^*\|^{1/p^k}, & \text{if } p > 1, \end{cases}$$
(37)

are the root-convergence factors of $\{\mathbf{x}^k\}$. The quantity

$$O_R(\mathbf{x}^*) = \begin{cases} \infty, & \text{if } R_p\{\mathbf{x}^k\} = 0, \forall p \in [1, \infty), \\ \inf\{p \in [1, \infty) | R_p\{\mathbf{x}^k\} = 1\}, & \text{otherwise,} \end{cases}$$
(38)

is called the root-convergence rate of $\{\mathbf{x}^k\}$.

We begin by proving that our method is locally convergent.

Theorem 1 Let the given eigenvalues $\{\lambda_i^*\}_{i=1}^n$ be distinct and $J(\mathbf{c}^*)$ defined in (19) be nonsingular. Then there exists $\delta > 0$ such that if $\|\mathbf{c}^0 - \mathbf{c}^*\| \leq \delta$, the sequence $\{\mathbf{c}^k\}$ generated by Algorithm II converges to \mathbf{c}^* .

Proof: Suppose that $\|\mathbf{c}^k - \mathbf{c}^*\| \leq \delta_1$, and $\|E_k\| \leq \epsilon = \min\{1, \epsilon_2\}$, where δ_1 and ϵ_2 are given in Lemma 5. By Lemmas 4 and 5, there exists a constant $\mu > 1$ such that for any $k \geq 0$,

$$\|\boldsymbol{\rho}^{k} - \boldsymbol{\lambda}^{*}\| \leq \mu(\|\mathbf{c}^{k} - \mathbf{c}^{*}\| + \|E_{k}\|), \qquad (39)$$

$$\|\mathbf{c}^{k+1} - \mathbf{c}^*\| \leq \mu(\|\boldsymbol{\rho}^k - \boldsymbol{\lambda}^*\|^\beta + \|E_k\|^2), \tag{40}$$

$$||E_{k+1}|| \leq \mu(||\mathbf{c}^{k+1} - \mathbf{c}^*|| + ||E_k||^2).$$
(41)

Putting (39) into (40), we have

$$\|\mathbf{c}^{k+1} - \mathbf{c}^*\| \leq \mu [\mu^{\beta} (\|\mathbf{c}^k - \mathbf{c}^*\| + \|E_k\|)^{\beta} + \|E_k\|^2]$$

$$\leq \mu [(2\mu)^{\beta} + 1] \max \{\|\mathbf{c}^k - \mathbf{c}\|^{\beta}, \|E_k\|^{\beta}\}.$$
(42)

Putting (42) into (41), and using the fact that $\mu > 1$, we have

$$||E_{k+1}|| \leq 2\mu \max \{ ||\mathbf{c}^{k+1} - \mathbf{c}||, ||E_k||^2 \}$$

$$\leq 2\mu^2 [(2\mu)^\beta + 1] \max \{ ||\mathbf{c}^k - \mathbf{c}||^\beta, ||E_k||^\beta \}.$$
(43)

Let $\varphi \equiv \max\{\tau_0 \sqrt{n}, 2\mu^2[(2\mu)^{\beta} + 1]\} > 1$. Then by (42) and (43), we have

$$\max\left\{\|\mathbf{c}^{k+1} - \mathbf{c}\|, \|E_{k+1}\|\right\} \le \varphi \max\left\{\|\mathbf{c}^k - \mathbf{c}\|^\beta, \|E_k\|^\beta\right\}, \quad k = 0, 1, \dots$$
(44)

We now prove the theorem by using the mathematical induction. In particular, we show that if $\|\mathbf{c}^0 - \mathbf{c}^*\| \le \delta$ where

$$\delta \equiv \min\left\{1, \delta_0, \delta_1, \frac{\epsilon}{\varphi}, \frac{1}{\varphi^{\beta^2/(\beta-1)^2}}\right\} < \epsilon,$$
(45)

then for each $k \ge 1$, the following inequalities hold:

$$\max\{\|\mathbf{c}^k - \mathbf{c}^*\|, \|E_k\|\} \leq \delta, \tag{46}$$

$$\max\{\|\mathbf{c}^{k}-\mathbf{c}^{*}\|,\|E_{k}\|\} \leq \varphi^{1+\beta+\dots+\beta^{k}}\|\mathbf{c}^{0}-\mathbf{c}^{*}\|^{\beta^{k}}.$$
(47)

We first note that from (20), we have

$$||E_0|| \le \sqrt{n} \max_i ||\mathbf{q}_i(\mathbf{c}^0) - \mathbf{q}_i(\mathbf{c}^*)|| \le \tau_0 \sqrt{n} ||\mathbf{c}^0 - \mathbf{c}^*|| \le \varphi ||\mathbf{c}^0 - \mathbf{c}^*||.$$
(48)

Hence by using (45), $||E_0|| \leq \varphi ||\mathbf{c}^0 - \mathbf{c}^*|| \leq \varphi \delta \leq \epsilon$.

We now verify (47) for k = 1. By (44) and (48),

$$\max\{\|\mathbf{c}^{1}-\mathbf{c}^{*}\|,\|E_{1}\|\} \leq \varphi \max\{\|\mathbf{c}^{0}-\mathbf{c}\|^{\beta},\|E_{0}\|^{\beta}\}$$
$$\leq \varphi\|\mathbf{c}^{0}-\mathbf{c}\|^{\beta}\max\{1,\varphi^{\beta}\}\leq \varphi^{1+\beta}\|\mathbf{c}^{0}-\mathbf{c}\|^{\beta}.$$
(49)

Moreover, if we define $\zeta \equiv \varphi^{\frac{\beta}{\beta-1}}\delta$, then by (45),

$$\zeta^{\beta} \le \delta. \tag{50}$$

Hence by (49),

$$\max\{\|\mathbf{c}^1 - \mathbf{c}^*\|, \|E_1\|\} \le \varphi^{1+\beta}\delta^{\beta} = (\varphi^{\frac{1+\beta}{\beta}}\delta)^{\beta} \le (\varphi^{\frac{\beta}{\beta-1}}\delta)^{\beta} = \zeta^{\beta} \le \delta$$

Thus (46) holds for k = 1.

Next we assume that at the kth iteration, (46) and (47) hold. We first prove that (47) holds for k + 1. In fact, by (44) and (47) for k, we have

$$\max\{\|\mathbf{c}^{k+1} - \mathbf{c}^*\|, \|E_{k+1}\|\} \leq \varphi \cdot \left(\varphi^{1+\beta+\dots+\beta^k}\|\mathbf{c}^0 - \mathbf{c}^*\|^{\beta^k}\right)^{\beta}$$
$$= \varphi^{1+\beta+\dots+\beta^{k+1}}\|\mathbf{c}^0 - \mathbf{c}^*\|^{\beta^{k+1}}.$$
(51)

To prove that (46) holds for k + 1, we use (51):

$$\max\{\|\mathbf{c}^{k+1} - \mathbf{c}^*\|, \|E_{k+1}\|\} \leq \left(\varphi^{\frac{1+\beta+\dots+\beta^k+\beta^{k+1}}{\beta^{k+1}}} \|\mathbf{c}^0 - \mathbf{c}^*\|\right)^{\beta^{k+1}}$$
$$= \left(\varphi^{\left(\frac{1}{\beta^{k+1}} + \frac{1}{\beta^k} + \dots + 1\right)} \|\mathbf{c}^0 - \mathbf{c}^*\|\right)^{\beta^{k+1}}$$
$$\leq \left(\varphi^{\frac{\beta}{\beta-1}} \|\mathbf{c}^0 - \mathbf{c}^*\|\right)^{\beta^{k+1}} \leq \zeta^{\beta^{k+1}}.$$
(52)

By (50), we have $\zeta \leq \delta^{1/\beta} \leq 1$. Hence

$$\max\{\|\mathbf{c}^{k+1} - \mathbf{c}^*\|, \|E_{k+1}\|\} \le \zeta^{\beta^{k+1}} \le \zeta^{\beta} \le \delta.$$
Thus we have proved that (46) and (47) hold for any $k \ge 1$. Moreover, from (52), we see that $\{\mathbf{c}^k\}$ converges to \mathbf{c}^* .

We end this section by establishing the root convergence of our method.

Theorem 2 Under the same conditions as in Theorem 1, the iterates $\{\mathbf{c}^k\}$ converges to \mathbf{c}^* with root-convergence rate at least equal to β .

Proof: By Theorem 1, we know that $\{\mathbf{c}^k\}$ converges to \mathbf{c}^* . From (52), we have for any $k \ge 1$, $\|\mathbf{c}^k - \mathbf{c}^*\| \le \zeta^{\beta^k}$, where $\zeta < 1$. We now estimate the root-convergence factors of $\{\mathbf{c}^k\}$ defined in (37) for different values of p:

1. If p = 1, then

$$R_1\{\mathbf{c}^k\} = \limsup_{k \to \infty} \|\mathbf{c}^k - \mathbf{c}^*\|^{1/k} \le \limsup_{k \to \infty} \zeta^{\beta^k/k} = 0.$$

2. If 1 , then

$$R_p\{\mathbf{c}^k\} = \limsup_{k \to \infty} \|\mathbf{c}^k - \mathbf{c}^*\|^{1/p^k} \le \limsup_{k \to \infty} \zeta^{(\beta/p)^k} = 0.$$

3. If $p = \beta$, then

$$R_{\beta}\{\mathbf{c}^k\} = \limsup_{k \to \infty} \|\mathbf{c}^k - \mathbf{c}^*\|^{1/\beta^k} \le \zeta < 1.$$

4. If $p > \beta$, then

$$R_p\{\mathbf{c}^k\} = \limsup_{k \to \infty} \|\mathbf{c}^k - \mathbf{c}^*\|^{1/p^k} \le \limsup_{k \to \infty} \zeta^{(\beta/p)^k} = 1.$$

Therefore, $R_p\{\mathbf{c}^k\} = 0$ for any $p \in [1, \beta)$ and $R_p\{\mathbf{c}^k\} \leq 1$ for any $p \in [\beta, \infty)$. Thus according to (38), $O_R(\mathbf{c}^*) \geq \beta$.

5 Numerical Experiments

In this section, we compare the numerical performance of Algorithm I with that of Algorithm II on two problems. The first one is the inverse Toeplitz eigenvalue problem, see [6, 27, 31], and the second one is the inverse Sturm-Liouville problem, see [14] and [8, p. 10]. Our aim is to illustrate the advantage of our method over Algorithm I in terms of minimizing the oversolving problem and the overall computational complexity.

Example 1. In this example, we use Toeplitz matrices as our A_i in (1):

$$A_{0} = O, A_{1} = I, A_{2} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix}, \dots, A_{n} = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & \ddots & \ddots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \ddots & \ddots & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Thus $A(\mathbf{c})$ is a symmetric Toeplitz matrix with first column equal to \mathbf{c} . We consider three problem sizes: n = 100, 200, and 300. For each value of n, we constructed ten n-by-n test problems where the exact solutions \mathbf{c}^* are chosen randomly. Then we computed the eigenvalues $\{\lambda_i^*\}_{i=1}^n$ of $A(\mathbf{c}^*)$ as the prescribed eigenvalues. Since both algorithms are locally convergent, \mathbf{c}^0 was formed by chopping the components of \mathbf{c}^* to four decimal places for n = 100 and to five decimal places for n = 200 and 300.

The linear systems (6), (10), (13), and (15) are solved iteratively by the QMR method [13] using the Matlab-provided QMR function. To guarantee the orthogonality of Q_k in (10) and P_k in (15), both systems are solved up to machine

precision eps (which is $\approx 2.2 \times 10^{-16}$). We use the right-hand side vector as the initial guess for these two systems.

For the Jacobian systems (6) and (13), we use \mathbf{c}^k , the iterant at the *k*th iteration, as the initial guess for the iterative method at the (k + 1)th iteration. We note that both systems are difficult to solve and one can use preconditioning to speed up the convergence. Here we have used the Matlab-provided Modified ILU (MILU) preconditioner: LUINC(A, [drop-tolerance,1,1,1]) since the MILU preconditioner is one of the most versatile preconditioners for unstructured matrices [9, 17]. The drop tolerance we used is 0.05 for all the three problem sizes. We emphasize that, we are not attempting to find the best preconditioners for these systems, but trying to illustrate that preconditioning can be incorporated into both systems easily.

The inner loop stopping tolerance for (13) is given by (14). For (6) in Algorithm I, we are supposed to solve it up to machine precision **eps**. Here however, we first try to solve (6) with a larger stopping tolerance of 10^{-13} and compare the two algorithms. Later we will vary this and see how it affects the performance of Algorithm I. The outer iterations of Algorithms I and II are stopped when

$$\|Q_k^T A(\mathbf{c}^k) Q_k - \Lambda_*\|_F \le 10^{-10}, \text{ and } \|P_k^T A(\mathbf{c}^k) P_k - \Lambda_*\|_F \le 10^{-10}.$$
 (53)

In Table 1, we give the total numbers of outer iterations N_o averaged over the ten tests and the average total numbers of inner iterations N_i required for solving the approximate Jacobian equations. In the table, "I" and "P" respectively mean

no preconditioner or the MILU preconditioner is used. We can see from Table 1 that N_o is small for Algorithm I and also for Algorithm II when $\beta \geq 1.5$. This confirms the theoretical convergence rate of the two algorithms. In terms of N_i , Algorithm II is more effective than Algorithm I for $\beta \approx 1.5$. We also note that the MILU preconditioner is quite effective for the Jacobian equations.

					β in Alg. II									
n			Alg. I	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	
100	Ι	N_o	3.2	12	5.2	4	3.3	3.2	3.2	3.2	3.2	3.2	3.2	
		N_i	397	755	445	379	327	323	325	329	336	339	349	
		N_o	3.2	7.7	5.3	4.2	3.7	3.2	3.2	3.2	3.2	3.2	3.2	
	Р	N_i	37.7	15.3	15.7	15.6	19	17.9	20.8	24	27.4	28.1	30.9	
200	Ι	N_o	3	10.9	6	4	3	3	3	3	3	3	3	
		N_i	818	1444	1144	855	684	719	725	732	738	747	763	
		No	3	7.4	5.1	4	3	3	3	3	3	3	3	
	Р	N_i	49.8	22.5	24.4	27.6	24.5	29.6	35.8	41	42.2	44	48.7	
300		N_o	3	11	6	4	3	3	3	3	3	3	3	
	1	N_i	1329	2086	1729	1348	1106	1171	1207	1241	1257	1259	1286	
		N_o	3	7.8	5.2	4	3	3	3	3	3	3	3	
	Р	N_i	74.2	35	35.7	37.3	32.9	40.2	48.4	56.1	62.3	65.4	67.5	

Table 1: Averaged total numbers of outer and inner iterations.

To further illustrate the oversolving problem, we give the convergence history of Algorithms I and II for one of the test matrices with n = 100 in Figure 1. The figure depicts the logarithm of the error versus the number of inner iterations for solving the Jacobian systems (6) and (13) by the preconditioned QMR method. We have labeled the error at the outer iterations with special symbols. We can see that for Algorithm I, the oversolving problem is very significant (see the horizontal lines between iteration numbers 5 to 15, and 20 to 28), whereas there are virtually no oversolving for Algorithm II with $\beta = 1.5$.



Figure 1: Convergence history of one of the test matrices.

In Table 1, (6) is solved with stopping tolerance $\eta = 10^{-13}$. One may expect that by increasing this stopping tolerance η , i.e. by solving (6) more inexactly, one can obtain an inexact method that may be better than our Algorithm II. To illustrate that it is not the case, we tried solving (6) with different η for ten matrices with n = 100 and 200, and compare their results with our Algorithm II with $\beta = 1.5$. We also repeated the experiments with four different iterative methods: the BiCG [32] and the CGS [30] methods together with their MILUpreconditioned versions. From Table 2, we see that our method is better than just solving (6) with increasing η . In fact, if η is big, the outer iteration does not converge within 20 iterations; and if η is small, the number of inner iterations will be bigger than that of our method. We also see that when n is larger, η should be smaller in order that the outer iteration converges. Also from Table 2, we see that CGS performs better than the other two iterative solvers if preconditioning is used, but is worse if not. Since in general, we do not have any information regarding the structure of the Jacobian matrix in (6) and (13), choosing a good iterative solver for these systems will not be an easy problem, not to mention the choice of an effective preconditioner for them. However, the results in Table 2 show that the oversolving problem is independent of the solvers we choose. Our method is always better than Algorithm I if the same iterative solver is used. Again MILU is an efficient preconditioner in all cases.

				n = 100		n = 200				
		Alg. II		Alş	g. I		Alg. II	Alg. I		
		$\beta = 1.5$	Stop	ping tole	cance η for	or (6)	$\beta = 1.5$	Stopping tolerance η for (6)		
			10^{-13}	10^{-12}	10^{-11}	10^{-10}		10^{-13}	10^{-12}	10^{-11}
No		3.2	3.2	3.2	3.2	> 20	3	3	3	> 20
QMR	N_i	323	397	356	344	*	719	818	738	*
BiCG	N_i	322	371	359	347	*	715	783	745	*
CGS	N_i	372	446	425	392	*	825	943	874	*
PQMR	N_i	17.9	37.7	32.7	28.2	*	29.6	49.8	41.8	*
PBiCG	N_i	18.3	37.7	33.1	28.5	*	30.5	49.5	42	*
PCGS	N_i	10.6	21.3	19	15.1	*	18.2	28.4	24.4	*

Table 2: Averaged total numbers of inner iterations.

As mentioned in §§2–3, solving the linear systems (10) and (15) iteratively will require only a few iterations since the coefficient matrices of these systems converge to the identity matrix as \mathbf{c}^k converges to \mathbf{c}^* . We report in Table 3 the numbers of iterations required for convergence for these systems, averaged over the ten test problems with n = 100 and 200. From the table, we see that the

number of inner iterations required is small and decreases as the outer iteration progresses. Thus it is reasonable to solve these systems by iterative solvers without any preconditioning.

	n = 100			n = 200			
Outer iteration	1 st	2nd	3rd	1 st	2nd	3rd	
Alg. I	9.7	5.4	2.6	8.6	4.8	2.0	
Alg. II with $\beta = 2.0$	9.8	5.3	2.6	8.6	4.8	2.0	
Alg. II with $\beta = 1.5$	9.9	5.3	2.6	8.5	4.7	2.0	

Table 3: Averaged numbers of inner iterations required by Step (d) of Algorithms I and II.

Example 2. Consider the Sturm-Liouville problem:

$$-u'' + q(x)u = \lambda u, \quad u(0) = u(\pi) = 0.$$
(54)

The inverse Sturm-Liouville problem is to determine q(x) from λ . By the central difference scheme with uniform mesh $h = \pi/(n+1)$, the differential equation (54) is reduced to the matrix eigenvalue problem with tridiagonal structure:

$$(A_0 + h^2 X) \mathbf{u} = h^2 \lambda \mathbf{u}, \tag{55}$$

where A_0 is the Laplacian matrix with zero boundary condition and X is a diagonal matrix representing the discretization of q(x).

The discrete analogue of the inverse Sturm-Liouville problem is an inverse eigenvalue problem. It is to determine the diagonal matrix X so that the matrix on the left hand side of (55) possesses a prescribed spectrum. Let $A_j = h^2 \mathbf{e}_j \mathbf{e}_j^T$, for $j = 1, \dots, n$, where \mathbf{e}_j is the *j*th unit *n*-vector. Thus we have the form (1) with $X = \operatorname{diag}(\mathbf{c})$. For demonstration purposes, we consider n = 100 here. Given the exact solution \mathbf{c}^* with entries $[\mathbf{c}^*]_i = e^{3ih}$, $1 \le i \le n$, i.e. $q(x) = e^{3x}$, we use the eigenvalues $\{h^2\lambda_i^*\}_{i=1}^n$ of $A(\mathbf{c}^*)$ as the prescribed spectrum. We perturb each entry of \mathbf{c}^* by a random number uniformly distributed between -1 and 1, and then use the perturbed vector as the initial guess \mathbf{c}^0 for both Algorithms I and II.

The systems (6), (10), (13), and (15) are solved by the MILU-preconditioned QMR method as in Example 1. Table 4 gives the total numbers of outer and inner iterations N_0 and N_i averaged over ten different initial guesses. From the table, we can see again that our method with $\beta \approx 1.5$ is better than Algorithm I.

	Alg. I	β in Alg. II									
		1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
N_o	3	7.8	5.3	4.4	4	3	3	3	3	3	3
N_i	71.6	65.1	60.3	60	62.8	48.6	56.6	60.4	65.7	68.1	73.2

Table 4: Averaged total numbers of outer and inner iterations for Example 2.

6 Remarks On Multiple Eigenvalues

In this section, we suppose that $\{\lambda_i^*\}_{i=1}^n$ includes multiple eigenvalues and that there exists a solution \mathbf{c}^* to IEP. For convenience, we assume that only the *s*th eigenvalue is multiple, with multiplicity t, i.e.,

$$\lambda_1^* < \lambda_2^* < \dots < \lambda_s^* = \lambda_{s+1}^* = \dots = \lambda_{s+t}^* < \lambda_{s+t+1}^* < \dots < \lambda_n^*.$$

Then it is easy to generalize our remarks to an arbitrary set of multiple eigenvalues.

Let us now consider Algorithm II. Equation (13) still holds, regardless of the eigenvalue multiplicities. The off-diagonal equations in Substep (c) of Step 2 is not true for $s \le i \ne j \le s + t$ as before. A reasonable course is to set

$$[Y_k]_{ij} = 0, \quad s \le i \ne j \le s+t$$

With this choice, following the proof of Theorems 1 and 2, we can show that the iterates $\{\mathbf{c}^k\}$ converge to \mathbf{c}^* with root-convergence rate at least β .

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The Solvability Conditions for the Inverse Eigenvalue Problem of Hermitian and Generalized Skew-Hamiltonian Matrices and Its Approximation

Abstract

In this paper, we first consider the inverse eigenvalue problem as follows: Find a matrix A with specified eigen-pairs, where A is a Hermitian and generalized skew-Hamiltonian matrix. The sufficient and necessary conditions are obtained, and a general representation of such a matrix is presented. We denote the set of such matrices by \mathcal{L}_S . Then the best approximation problem for the inverse eigenproblem is discussed. That is: Given an arbitrary \tilde{A} , find a matrix $A^* \in \mathcal{L}_S$ which is nearest to \tilde{A} in the Frobenius norm. We show that the best approximation is unique and provide an expression for this nearest matrix.

1 Introduction

Let $J \in \mathbb{R}^{n \times n}$ be an orthogonal skew-symmetric matrix, i.e. $J \in \mathbb{R}^{n \times n}$ satisfies that $J^T J = J J^T = I_n$, $J^T = -J$. Then we have $J^2 = -I_n$ and $n = 2k, k \in N$. In the following, we give the definitions of generalized Hamiltonian and general**Definition 1** Given an orthogonal skew-symmetric matrix J.

- (1) A matrix $H \in \mathbb{C}^{n \times n}$ is called generalized Hamiltonian if $(HJ)^H = HJ$. The set of all n-by-n generalized Hamiltonian matrices is denoted by $\mathbb{GH}^{n \times n}$.
- (2) A matrix $H \in \mathbb{C}^{n \times n}$ is called generalized skew-Hamiltonian if $(HJ)^H = -HJ$. The set of all n-by-n generalized skew-Hamiltonian matrices is denoted by $\mathbb{GSH}^{n \times n}$.

We observe that the sets $\mathbb{GH}^{n \times n}$ and $\mathbb{GSH}^{n \times n}$ depend on the choice of the matrix J. If $J = \begin{bmatrix} 0 & I_k \\ -I_k & 0 \end{bmatrix}$, then the sets $\mathbb{GH}^{n \times n}$ and $\mathbb{GSH}^{n \times n}$ are the well-known sets of Hamiltonian and skew-Hamiltonian matrices.

Definition 2 Given an orthogonal skew-symmetric matrix J.

- A matrix A ∈ C^{n×n} is said to be a Hermitian and generalized Hamiltonian matrix if A^H = A and (AJ)^H = AJ. The set of all n-by-n Hermitian and generalized Hamiltonian matrices is denoted by HH^{n×n}.
- (2) A matrix A ∈ C^{n×n} is said to be a Hermitian and generalized skew-Hamiltonian matrix if A^H = A and (AJ)^H = −AJ. The set of all n-by-n Hermitian and generalized skew-Hamiltonian matrices is denoted by HSH^{n×n}.

Hamiltonian and skew-Hamiltonian matrices play an important role in engineering, such as in linear-quadratic optimal control [13, 17], H_{∞} optimization [24], and the related problem of solving algebraic Riccati equations [11].

In this paper, we will study two problems related to Hermitian and generalized skew-Hamiltonian matrices. The first problem is a kind of inverse eigenvalue problems. For decades, structured inverse eigenvalue problems have been of great value for many applications, see for instance the expository papers [7, 22]. There are also different types of inverse eigenproblem, for instances multiplicative type and additive type [22, Chapter 4]. In what follows, we consider the following type of inverse eigenproblem which appeared in the design of Hopfield neural networks [6, 12].

Problem I. Given $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m] \in \mathbb{C}^{n \times m}$ and $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_m) \in \mathbb{C}^{m \times m}$, find a Hermitian and generalized skew-Hamiltonian matrix A in $\mathbb{HSH}^{n \times n}$ such that $AX = X\Lambda$.

We note from the above definition that the eigenvalues of a Hermitian and generalized skew-Hamiltonian matrix are real numbers. Hence we have $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m) \in \mathbb{R}^{m \times m}$.

The second problem we consider in this paper is the problem of best approximation:

Problem II. Let \mathcal{L}_S be the solution set of Problem I. Given a matrix $\tilde{A} \in \mathbb{C}^{n \times n}$, find $A^* \in \mathcal{L}_S$ such that

$$\|\tilde{A} - A^*\| = \min_{A \in \mathcal{L}_S} \|\tilde{A} - A\|,$$

where $\|\cdot\|$ is the Frobenius norm.

The best approximation problem occurs frequently in experimental design, see for instance [14, p.123]. Here the matrix \tilde{A} may be a matrix obtained from experiments, but it may not satisfy the structural requirement (Hermitian and generalized skew-Hamiltonian) and/or spectral requirement (having eigenpairs Xand Λ). The best estimate A^* is the matrix that satisfies both restrictions and is the best approximation of \tilde{A} in the Frobenius norm, see for instance [2, 3, 10].

Problems I and II have been solved for different classes of structured matrices, see for instance [21, 23]. In this paper, we extend the results in [23] to the class of Hermitian and generalized skew-Hamiltonian matrices. We first give a solvability condition for Problem I and also the form of its general solution. Then in the case when Problem I is solvable, we show that Problem II has a unique solution and give a formula for the minimizer A^* .

In this paper, the notations are as follows. Let $\mathcal{U}(n)$ be the set of all *n*-by-*n* unitary matrices, and $\mathbb{H}^{n \times n}$ denote the set of all *n*-by-*n* Hermitian matrices. We denote the transpose, conjugate transpose and the Moore-Penrose generalized inverse of a matrix A by A^T , A^H and A^+ respectively, and the identity matrix of order *n* by I_n . We define the inner product in space $\mathbb{C}^{n \times m}$ by

$$(A, B) = \operatorname{tr}(A^H B), \quad \forall A, B \in \mathbb{C}^{n \times m}$$

Then $\mathbb{C}^{n \times m}$ is a Hilbert inner product space. The norm of a matrix generated by the inner product space is the Frobenius norm.

This paper is outlined as follows. In §2 we first discuss the structure of the set $\mathbb{HSH}^{n \times n}$, and then present the solvability conditions and provide the general solution formula for Problem I. In §3 we first show the existence and uniqueness

of the solution for Problem II, and then derive an expression of the solution when the solution set \mathcal{L}_S is nonempty, and finally propose an algorithm to compute the solution to Problem II. In §4 we give some illustrative numerical examples.

2 Solvability Conditions of Problem I

We first discuss the structure of $\mathbb{HSH}^{n \times n}$. In what follows, we always assume that $n = 2k, k \in N$. By the definition of $\mathbb{HSH}^{n \times n}$, we have the following statement.

Lemma 1 Let $A \in \mathbb{C}^{n \times n}$, then $A \in \mathbb{HSH}^{n \times n}$ if and only if $A^H = A$, AJ - JA = 0.

Since J is orthogonal skew-symmetric, J is normal and skew-symmetric and then has only two multiple eigenvalues i and -i with multiplicity k respectively, where i denotes the the imaginary unit, i.e. $i^2 = -1$. Thus we can easily show the following lemma.

Lemma 2 Let $J \in \mathbb{R}^{n \times n}$ be orthogonal skew-symmetric, then there exists a matrix $U \in \mathcal{U}(n)$ such that

$$J = U \begin{bmatrix} i \cdot I_k & 0 \\ 0 & -i \cdot I_k \end{bmatrix} U^H.$$
(1)

By the above two lemmas, we have the following result for the structure of $\mathbb{HSH}^{n \times n}$.

Theorem 1 Let $A \in \mathbb{C}^{n \times n}$ and the spectral decomposition of J be given as (1). Then $A \in \mathbb{HSH}^{n \times n}$ if and only if

$$A = U \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} U^{H}, \quad A_{11}, A_{22} \in \mathbb{H}^{k \times k}.$$
 (2)

Proof: If $A \in \mathbb{HSH}^{n \times n}$, then by Lemma 1 and (1), we obtain

$$U^{H}AU\begin{bmatrix}i\cdot I_{k} & 0\\ 0 & -i\cdot I_{n-k}\end{bmatrix} + \begin{bmatrix}i\cdot I_{k} & 0\\ 0 & -i\cdot I_{n-k}\end{bmatrix} U^{H}AU = 0.$$
(3)

Since $A^{H} = A$, then $U^{H}AU \in \mathbb{H}^{n \times n}$. Let

$$A = U \begin{bmatrix} A_{11} & A_{12} \\ & & \\ A_{12}^H & A_{22} \end{bmatrix} U^H, \quad A_{11} \in \mathbb{H}^{k \times k}, A_{22} \in \mathbb{H}^{k \times k}.$$

Substituting it into (3) yields (2).

On the other hand, if A can be expressed as (2), then, obviously, $A^H = A$, AJ - JA = 0. By Lemma 1, $A \in \mathbb{HSH}^{n \times n}$.

We now investigate the solvability of Problem I. We need the following lemma, see for instance [19].

Lemma 3 [19, Lemma 1.4] Let $B, C \in \mathbb{C}^{n \times m}$ be given. Then HB = C has a solution in $\mathbb{H}^{n \times n}$ if and only if

$$C = CB^+B \quad and \quad (BB^+CB^+)^H = BB^+CB^+.$$

In this case the general solution can be expressed by

$$Y = CB^{+} + (B^{+})^{H}C^{H} - (B^{+})^{H}C^{H}BB^{+} + (I - BB^{+})Z(I - BB^{+}),$$

where $Z \in \mathbb{H}^{n \times n}$ is arbitrary.

Then we can establish the solvability of Problem I as follows.

Theorem 2 Given $X \in \mathbb{C}^{n \times m}$, $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m) \in \mathbb{R}^{m \times m}$. Let

$$U^{H}X = \begin{bmatrix} \tilde{X}_{1} \\ \tilde{X}_{2} \end{bmatrix}, \quad \tilde{X}_{1}, \tilde{X}_{2} \in \mathbb{C}^{k \times m}.$$
(4)

Then there exists $A \in \mathbb{HSH}^{n \times n}$ such that $AX = X\Lambda$ if and only if

$$\tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_1 \Lambda, \quad (\tilde{X}_1^+)^H \Lambda (\tilde{X}_1^+)^H = \tilde{X}_1 \Lambda \tilde{X}_1^+,$$
(5)

and

$$\tilde{X}_2 \Lambda \tilde{X}_2^+ \tilde{X}_2 = \tilde{X}_2 \Lambda, \quad (\tilde{X}_2^+)^H \Lambda (\tilde{X}_2^+)^H = \tilde{X}_2 \Lambda \tilde{X}_2^+.$$
(6)

In this case the general solution is given by

$$A = A_0 + U \begin{bmatrix} (I_k - \tilde{X}_1 \tilde{X}_1^+) Z_1 (I_k - \tilde{X}_1 \tilde{X}_1^+) & 0\\ 0 & (I_k - \tilde{X}_2 \tilde{X}_2^+) Z_2 (I_k - \tilde{X}_2 \tilde{X}_2^+) \end{bmatrix} U^H, \quad (7)$$

where Z_1 and $Z_2 \in \mathbb{H}^{k \times k}$ are arbitrary and

$$A_0 = U \begin{bmatrix} \tilde{X}_1 \Lambda \tilde{X}_1^+ & 0\\ 0 & \tilde{X}_2 \Lambda \tilde{X}_2^+ \end{bmatrix} U^H.$$
 (8)

Proof: We assume that A is a solution to Problem I. By Theorem 1, there is a solution to Problem I if and only if there exist $A_{11}, A_{22} \in \mathbb{H}^{k \times k}$ such that

$$A = U \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} U^H, \quad AX = X\Lambda,$$

i.e.

$$U\begin{bmatrix} A_{11} & 0\\ 0 & A_{22} \end{bmatrix} U^H X = X\Lambda.$$
 (9)

(9) is equivalent to

$$A_{11}\tilde{X}_1 = \tilde{X}_1\Lambda \quad \text{and} \quad A_{22}\tilde{X}_2 = \tilde{X}_2\Lambda.$$
(10)

By Lemma 3, (10) have solutions in $\mathbb{H}^{n \times n}$ if and only if

$$\tilde{X}_{1}\Lambda\tilde{X}_{1}^{+}\tilde{X}_{1} = \tilde{X}_{1}\Lambda, \quad (\tilde{X}_{1}\tilde{X}_{1}^{+}\tilde{X}_{1}\Lambda\tilde{X}_{1}^{+})^{H} = \tilde{X}_{1}\tilde{X}_{1}^{+}\tilde{X}_{1}\Lambda\tilde{X}_{1}^{+}, \tag{11}$$

and

$$\tilde{X}_{2}\Lambda\tilde{X}_{2}^{+}\tilde{X}_{2} = \tilde{X}_{2}\Lambda, \quad (\tilde{X}_{2}\tilde{X}_{2}^{+}\tilde{X}_{2}\Lambda\tilde{X}_{2}^{+})^{H} = \tilde{X}_{2}\tilde{X}_{2}^{+}\tilde{X}_{2}\Lambda\tilde{X}_{2}^{+}.$$
(12)

Since $\tilde{X}_1 \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_1$ and $\tilde{X}_2 \tilde{X}_2^+ \tilde{X}_2 = \tilde{X}_2$, (11) and (12) are equivalent to (5) and (6) respectively. Moreover in this case, the general solutions to (10) is given by

$$A_{11} = \tilde{X}_1 \Lambda \tilde{X}_1^+ + (\tilde{X}_1^+)^H \Lambda \tilde{X}_1^H - (\tilde{X}_1^+)^H \Lambda \tilde{X}_1^H \tilde{X}_1 \tilde{X}_1^+$$
(13)
+ $(I_k - \tilde{X}_1 \tilde{X}_1^+) Z_1 (I_k - \tilde{X}_1 \tilde{X}_1^+)$

$$= \tilde{X}_1 \Lambda \tilde{X}_1^+ + (I_k - \tilde{X}_1 \tilde{X}_1^+) Z_1 (I_k - \tilde{X}_1 \tilde{X}_1^+), \qquad (14)$$

$$A_{22} = \tilde{X}_2 \Lambda \tilde{X}_2^+ + (\tilde{X}_2^+)^H \Lambda \tilde{X}_2^H - (\tilde{X}_2^+)^H \Lambda \tilde{X}_2^H \tilde{X}_2 \tilde{X}_2^+$$
(15)

$$+ (I_k - \tilde{X}_2 \tilde{X}_2^+) Z_2 (I_k - \tilde{X}_2 \tilde{X}_2^+)$$

= $\tilde{X}_2 \Lambda \tilde{X}_2^+ + (I_k - \tilde{X}_2 \tilde{X}_2^+) Z_2 (I_k - \tilde{X}_2 \tilde{X}_2^+),$ (16)

where $Z_1, Z_2 \in \mathbb{H}^{k \times k}$ is arbitrary. Let

$$A_0 = U \begin{bmatrix} \tilde{X}_1 \Lambda \tilde{X}_1^+ & 0 \\ 0 & \tilde{X}_2 \Lambda \tilde{X}_2^+ \end{bmatrix} U^H.$$

Substituting (13) into (2) gives rise to (7).

3 The Solution to Problem II

In this section, we solve Problem II over \mathcal{L}_S when \mathcal{L}_S is nonempty. We first recall the following statement.

Lemma 4 [8, Theorem 2] Let $E, H \in \mathbb{C}^{n \times n}$. If $H \in \mathbb{H}^{n \times n}$, then

$$||E - \frac{E + E^H}{2}|| \le ||E - H||.$$

Then we have the following theorem for the solution to Problem II over \mathcal{L}_S .

Theorem 3 Given $\tilde{A} \in \mathbb{C}^{n \times n}$, $X \in \mathbb{C}^{n \times m}$, and the notation of X, Λ and conditions are the same as in Theorem 2. Let

$$U^{H}\tilde{A}U = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix}, \quad \tilde{A}_{11}, \tilde{A}_{22} \in \mathbb{C}^{k \times k}.$$
 (17)

If \mathcal{L}_S is nonempty, then Problem II has a unique solution A^* and A^* can be represented as

$$A^* = A_0 + U \begin{bmatrix} P(\frac{\tilde{A}_{11} + \tilde{A}_{11}^H}{2})P & 0\\ 0 & Q(\frac{\tilde{A}_{22} + \tilde{A}_{22}^H}{2})Q \end{bmatrix} U^H,$$
 (18)

where A_0 is given by (8) and

$$P = I_k - \tilde{X}_1 \tilde{X}_1^+, \quad Q = I_k - \tilde{X}_2 \tilde{X}_2^+.$$
(19)

Proof: When \mathcal{L}_S is nonempty, it is easy to verify from (7) that \mathcal{L}_S is a closed convex set. Since $\mathbb{C}^{n \times n}$ is a uniformly convex Banach space under the Frobenius norm, there exists a unique solution for Problem II [5, p. 22]. Because the Frobenius norm is unitary invariant, Problem II is equivalent to

$$\min_{A \in \mathcal{L}_S} \| U^H \tilde{A} U - U^H A U \|^2.$$
(20)

By Theorem 2, we have

$$\|U^{H}\tilde{A}U - U^{H}AU\|^{2} = \left\| \begin{bmatrix} \tilde{A}_{11} - \tilde{X}_{1}\Lambda\tilde{X}_{1}^{+} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} - \tilde{X}_{2}\Lambda\tilde{X}_{2}^{+} \end{bmatrix} - \begin{bmatrix} PZ_{1}P & 0 \\ 0 & QZ_{2}Q \end{bmatrix} \right\|^{2}$$

Thus (20) is equivalent to

$$\min_{Z_1 \in \mathbb{H}^{k \times k}} \|\tilde{A}_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+ - P Z_1 P\|^2 + \min_{Z_2 \in \mathbb{H}^{k \times k}} \|\tilde{A}_{22} - \tilde{X}_2 \Lambda \tilde{X}_2^+ - Q Z_2 Q\|^2.$$

By Lemma 4, the solution is given by Z_1^* and Z_2^* such that

$$PZ_1^*P = \frac{\tilde{A}_{11} + \tilde{A}_{11}^H}{2} - \tilde{X}_1\Lambda\tilde{X}_1^+,$$
$$QZ_2^*Q = \frac{\tilde{A}_{22} + \tilde{A}_{22}^H}{2} - \tilde{X}_2\Lambda\tilde{X}_2^+.$$

Notice from (19) that P and Q are projection matrices, i.e. $P^2 = P$ and $Q^2 = Q$. Therefore $PZ_1^*P = P(\frac{\tilde{A}_{11}+\tilde{A}_{11}^H}{2}-\tilde{X}_1\Lambda\tilde{X}_1^+)P$ and $QZ_2^*Q = Q(\frac{\tilde{A}_{22}+\tilde{A}_{22}^H}{2}-\tilde{X}_2\Lambda\tilde{X}_2^+)Q$. Let $G_{11} = \frac{\tilde{A}_{11}+\tilde{A}_{11}^H}{2}$. Notice further that because $\tilde{X}_1^+\tilde{X}_1\tilde{X}_1^+ = \tilde{X}_1^+$, we have

$$P(G_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+)P = P(G_{11} - G_{11} \tilde{X}_1 \tilde{X}_1^+ - \tilde{X}_1 \Lambda \tilde{X}_1^+ + \tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 \tilde{X}_1^+)$$

= $P(G_{11} - G_{11} \tilde{X}_1 \tilde{X}_1^+) = PG_{11}P.$

That is, $PZ_1^*P = P(\frac{\tilde{A}_{11}+\tilde{A}_{11}^H}{2})P$. Similarly, $QZ_2^*Q = Q(\frac{\tilde{A}_{22}+\tilde{A}_{22}^H}{2})Q$. Hence the unique solution for Problem II is given by (18).

Based on Theorem 3, we propose the following algorithm for solving Problem II over \mathcal{L}_S .

Algorithm I

- (1) Compute \tilde{X}_1 and \tilde{X}_2 by (4).
- (2) Compute \tilde{X}_1^+ and \tilde{X}_2^+ .
- (3) If

$$\tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_1 \Lambda, \quad (\tilde{X}_1^+)^H \Lambda (\tilde{X}_1)^H = \tilde{X}_1 \Lambda \tilde{X}_1^+,$$

and

$$\tilde{X}_2\Lambda\tilde{X}_2^+\tilde{X}_2 = \tilde{X}_2\Lambda, \quad (\tilde{X}_2^+)^H\Lambda(\tilde{X}_2)^H = \tilde{X}_2\Lambda\tilde{X}_2^+,$$

then the solution set \mathcal{L}_S to Problem I is nonempty and we continue. Otherwise we stop.

- (4) Compute \tilde{A}_{11} and \tilde{A}_{22} by (17).
- (5) Compute $G_{11} = \frac{\tilde{A}_{11} + \tilde{A}_{11}^H}{2}$ and $G_{22} = \frac{\tilde{A}_{22} + \tilde{A}_{22}^H}{2}$.
- (6) Compute

$$M_{11} = \tilde{X}_1 \Lambda \tilde{X}_1^+ + G_{11} - G_{11} \tilde{X}_1 \tilde{X}_1^+ - \tilde{X}_1 \tilde{X}_1^+ G_{11} - \tilde{X}_1 \tilde{X}_1^+ G_{11} \tilde{X}_1 \tilde{X}_1^+,$$

$$M_{22} = \tilde{X}_2 \Lambda \tilde{X}_2^+ + G_{22} - G_{22} \tilde{X}_2 \tilde{X}_2^+ - \tilde{X}_2 \tilde{X}_2^+ G_{22} + \tilde{X}_2 \tilde{X}_2^+ G_{22} \tilde{X}_2 \tilde{X}_2^+.$$

(7) Compute $A^* = U \begin{bmatrix} M_{11} & 0 \\ 0 & M_{22} \end{bmatrix} U^H.$

Now, we consider the computational complexity of our algorithm. We observe from Lemma 2 that, for different choice of J, the structure of $U \in \mathcal{U}(n)$ may be varied. Thus the total computational complexity may be changed.

We first consider the case when given a fixed J with $U \in \mathcal{U}(n)$ dense. For Step (1), since U is dense, it requires $O(n^2m)$ operations to compute \tilde{X}_1 and \tilde{X}_2 . For Step (2), using singular value decomposition to compute \tilde{X}_1^+ and \tilde{X}_2^+ requires $O(n^2m + m^3)$ operations. Step (3) obviously requires $O(n^2m)$ operations. For Step(4), because of the density of U, the operations required is $O(n^3)$. Step(5) requires O(n) operations only. For Step(6), if we compute $G_{ii}\tilde{X}_i\tilde{X}_i^+$ as $[(G_{ii}\tilde{X}_i)\tilde{X}_i^+]$, $\tilde{X}_i\tilde{X}_i^+G_{ii}$ as $[\tilde{X}_i(\tilde{X}_i^+G_{ii})]$, and $\tilde{X}_i\tilde{X}_i^+G_{ii}\tilde{X}_i\tilde{X}_i^+$ as $\{\tilde{X}_i[(\tilde{X}_i^+(G_{ii}\tilde{X}_i))\tilde{X}_i^+]\}$, then the cost will only be of $O(n^2m)$ operations. Finally, because of the density of Uagain, Step (7) requires $O(n^3)$ operations. Thus the total cost of the algorithm is $O(n^3 + n^2m + m^3)$. In particular, if we choose that

$$J = \begin{bmatrix} 0 & I_k \\ & \\ -I_k & 0 \end{bmatrix}, \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix} I_k & I_k \\ i \cdot I_k & -i \cdot I_k \end{bmatrix} \in \mathcal{U}(n)$$

Then, because of the sparsity of U, Steps (1), (4) and (7) will require O(nm), $O(n^2)$ and $O(n^2)$ respectively. Therefore the total complexity of the algorithm is $O(n^2m + m^3)$.

Finally, we remark that in practice, $m \ll n$. In addition, it is easy to verify that our algorithm is stable.

4 Numerical Experiments

In this section, we will give some numerical examples to illustrate our results. All the tests are performed by MATLAB which has a machine precision around 10^{-16} . In the following, we let $n = 2k, k \in N$ and $J = \begin{bmatrix} 0 & I_k \\ -I_k & 0 \end{bmatrix}$. Then it is clear that the spectral decomposition of J is given by

$$\begin{bmatrix} i \cdot I_k & 0 \end{bmatrix}$$

$$J = U \begin{bmatrix} & & \\ & 0 & -i \cdot I_k \end{bmatrix} U^H,$$

where $U = \frac{1}{\sqrt{2}} \begin{bmatrix} I_k & I_k \\ i \cdot I_k & -i \cdot I_k \end{bmatrix}$, $U^H U = U U^H = I_n$.

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Example 1. We choose a random matrix A in $\mathbb{HSH}^{n \times n}$:

$$A = \begin{bmatrix} 1.9157 & -0.5359 + 5.5308i & 0 + 0.0596i & 4.2447 + 0.1557i \\ -0.5359 - 5.5308i & -0.5504 & -4.2447 + 0.1557i & 0 + 0.8957i \\ 0 - 0.0596i & -4.2447 - 0.1557i & 1.9157 & -0.5359 + 5.5308i \\ 4.2447 - 0.1557i & 0 - 0.8957i & -0.5359 - 5.5308i & -0.5504 \end{bmatrix}$$

Then the eigenvalues of A are -9.7331, -0.4090, 2.7296, and 10.1431. We let $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$ denote the eigenvectors of A associated with -9.7331, -0.4090, 2.7296, and 10.1431 respectively. Now we take $X = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4]$, i.e.

$$X = \begin{bmatrix} -0.4554 - 0.0322i & 0.3324 + 0.0983i & 0.5910 + 0.1747i & 0.5386 + 0.0381i \\ 0.0000 - 0.5399i & -0.0000 + 0.6163i & -0.0000 - 0.3466i & 0.0000 - 0.4566i \\ 0.0322 - 0.4554i & 0.0983 - 0.3324i & 0.1747 - 0.5910i & -0.0381 + 0.5386i \\ 0.5399 & 0.6163 & -0.3466 & 0.4566 \end{bmatrix}$$

and

$$\Lambda = \begin{vmatrix} -9.7331 & 0 & 0 & 0 \\ 0 & -0.4090 & 0 & 0 \\ 0 & 0 & 2.7296 & 0 \\ 0 & 0 & 0 & 10.1431 \end{vmatrix}$$

Given such X and Λ , it is easy to see that there exists a solution for Problem I, i.e. A. Thus \mathcal{L}_S is nonempty. If we perturb A to obtain a matrix $\tilde{A}(\epsilon) = A + \epsilon \cdot C \notin \mathbb{HSH}^{n \times n}$, where

$$C = \begin{bmatrix} 0.2476 + 0.7668i & 0.3006 + 0.8790i & 0.8569 + 0.4963i & 0.2968 + 0.3608i \\ 0.4358 + 0.5740i & 0.2659 + 0.9058i & 0.2429 + 0.3921i & 0.3903 + 0.3135i \\ 0.9776 + 0.7098i & 0.1334 + 0.0886i & 0.1949 + 0.5583i & 0.1873 + 0.7436i \\ 0.8600 + 0.8126i & 0.7425 + 0.3055i & 0.3908 + 0.6318i & 0.8957 + 0.2838i \end{bmatrix}$$

then the conditions in Theorem 2 and Theorem 3 are satisfied. Using Algorithm I in §3, we get the solution $A^*(\epsilon)$ of Theorem 3 corresponding to $\tilde{A}(\epsilon)$. In Figure 1, we plot the following two quantities for ϵ from 10^{-10} to 10^{10} : $\log_{10} \|\tilde{A}(\epsilon) - A^*(\epsilon)\|$



Figure 1: $\log_{10} \|\tilde{A}(\epsilon) - A^*(\epsilon)\|$ ("+") and $\log_{10} \|A - A^*(\epsilon)\|$ ("*") versus $\log_{10} \epsilon$ for Example 1.

(marked by "+") and $\log_{10} ||A - A^*(\epsilon)||$ (marked by "*"). We observe from Figure 1 that $A^*(\epsilon)$ approaches gradually $\tilde{A}(\epsilon)$ as ϵ goes to zero. While for any ϵ between 10^{-10} and 10^{10} , $A^*(\epsilon) = A$ almost up to the machine precision.

Example 2. We solve Problems I and II with multiple eigenvalues. The following is one of various eigenpairs we have tested:

$$X = \begin{bmatrix} 0.0553 + 0.2344i & 0.1528 + 0.6470i & 0.2859 + 0.3281i & 0.3662 + 0.4202i \\ -0.6648 & 0.2408 & -0.5573 & 0.4352 \\ -0.2344 + 0.0553i & -0.6470 + 0.1528i & 0.3281 - 0.2859 & 0.4202 - 0.3662i \\ 0 - 0.6648i & 0 + 0.2408i & 0 + 0.5573i & 0 - 0.4352i \end{bmatrix}$$

and

$$\Lambda = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

Given such X and Λ , it is easy to verify that there exists a solution for Problem I, i.e.

$$A = \begin{bmatrix} 1.1946 & 0.2329 + 0.4945i & 0 + 0.4266i & 0.1288 + 0.0858i \\ 0.2329 - 0.4945i & 0.3054 & -0.1288 + 0.0858i & 0 + 1.0734i \\ 0 - 0.4266i & -0.1288 - 0.0858i & 1.1946 & 0.2329 + 0.4945i \\ 0.1288 - 0.0858i & 0 - 1.0734i & 0.2329 - 0.4945i & 0.3054 \end{bmatrix}$$

Thus \mathcal{L}_S is nonempty. We now perturb A to obtain a matrix $\tilde{A}(\epsilon) = A + \epsilon \cdot F \notin \mathbb{HSH}^{n \times n}$, where

$$F = \begin{bmatrix} 0.8408 + 0.4910i & 0.7168 + 0.5550i & 0.9106 + 0.6066i & 0.8739 + 0.6959i \\ 0.6463 + 0.9427i & 0.8112 + 0.5147i & 0.2761 + 0.3202i & 0.7105 + 0.7889i \\ 0.0559 + 0.5107i & 0.1534 + 0.7272i & 0.9571 + 0.4688i & 0.9746 + 0.9407i \\ 0.2057 + 0.3490i & 0.0864 + 0.1896i & 0.7400 + 0.7850i & 0.1543 + 0.6763i \end{bmatrix}$$

Then the conditions in Theorems 2 and 3 are satisfied. Using Algorithm I in §3, we get the solution $A^*(\epsilon)$ of Theorem 3 corresponding to $\tilde{A}(\epsilon)$. In Figure 2, we plot the following two quantities for ϵ from 10^{-10} to 10^{10} : $\log_{10} \|\tilde{A}(\epsilon) - A^*(\epsilon)\|$ (marked by "+") and $\log_{10} \|A - A^*(\epsilon)\|$ (marked by "*"). We can see from Figure 2 that $A^*(\epsilon)$ approximates to $\tilde{A}(\epsilon)$ as ϵ goes to zero. However, for any ϵ between 10^{-10} and 10^{10} , $A^*(\epsilon) = A$ almost up to the machine precision.

Example 3. Let T(1:n) denote a *n*-by-*n* Hermitian Toeplitz matrix whose first row is $(1, 2+2 \cdot i, \ldots, n+n \cdot i)$, and T(1:1/n) be a *n*-by-*n* Hermitian Toeplitz



Figure 2: $\log_{10} \|\tilde{A}(\epsilon) - A^*(\epsilon)\|$ ("+") and $\log_{10} \|A - A^*(\epsilon)\|$ ("*") versus $\log_{10} \epsilon$ for Example 2.

matrix whose first row is $(1, 1/2 + 1/2 \cdot i, \dots, 1/n + 1/n \cdot i)$. For example

$$T(1:4) = \begin{bmatrix} 1 & 2+2i & 3+3i & 4+4i \\ 2-2i & 1 & 2+2i & 3+3i \\ 3-3i & 2-2i & 1 & 2+2i \\ 4-4i & 3-3i & 2-2i & 1 \end{bmatrix}$$

,

and

$$T(1:1/4) = \begin{bmatrix} 1 & 1/2 + 1/2i & 1/3 + 1/3i & 1/4 + 1/4i \\ 1/2 - 1/2i & 1 & 1/2 + 1/2i & 1/3 + 1/3i \\ 1/3 - 1/3i & 1/2 - 1/2i & 1 & 1/2 + 1/2i \\ 1/4 - 1/4i & 1/3 - 1/3i & 1/2 - 1/2i & 1 \end{bmatrix}$$

By Theorem 1, if

$$A = U \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} U^{H}, \quad A_{11}, A_{22} \in \mathbb{H}^{n \times n},$$

k	A_{11}	A_{22}	$\ \Delta A\ = \ \tilde{A} - A^*\ $	Time (s)
25	T(1:25)	T(1:1/25)	0.2930	0.1300
50	T(1:50)	T(1:1/50)	0.8226	0.6500
100	T(1:100)	T(1:1/100)	2.3181	4.3300
150	T(1:150)	T(1:1/150)	4.2532	13.6500
200	T(1:200)	T(1:1/200)	6.5442	31.2800

Table 1: Numerical results for Example 3.

then $A \in \mathbb{HSH}^{n \times n}$. We assume that λ_j, \mathbf{x}_j are eigenpairs of A. Now we take $X = [\mathbf{x}_1, \dots, \mathbf{x}_n], \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$. Let $\tilde{A} = A + \Delta A, \Delta A = 10^{-3} \cdot C$, where C is a complex matrix of order n whose first column is $(1, 2, \dots, n)^T$ and whose first row is $(1, 2 \cdot i, \dots, n \cdot i)$ and the other entries are zeros. Then the Frobenius norm of ΔA becomes larger as n increases. We can theoretically show that A^* approaches to A as the rank of X is greater. In particular, when the rank of X is n, it is clear that $A^* = A$. We take $A_{11} = T(1:k)$ and $A_{22} = T(1:1/k)$. We test Algorithm I in §3 using MATLAB 6.1.

In Table 1, we list our numerical results, where 'Time' is the CPU timings.

The above three examples and many other examples we have tested by MAT-LAB confirm our theoretical results in this paper. We also note from the numerical experiments that as \tilde{A} approximates a solution of Problem I, \tilde{A} becomes closer to the unique solution A^* of Problem II. This also agrees with our prediction.

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Inverse Eigenproblems for Centrosymmetric and Centroskew Matrices and Their Approximation

Abstract

In this paper, we first give the solvability condition for the following inverse eigenproblem (IEP): given a set of vectors $\{\mathbf{x}_i\}_{i=1}^m$ in \mathbb{C}^n and a set of complex numbers $\{\lambda_i\}_{i=1}^m$, find a centrosymmetric or centroskew matrix Cin $\mathbb{R}^{n \times n}$ such that $\{\mathbf{x}_i\}_{i=1}^m$ and $\{\lambda_i\}_{i=1}^m$ are the eigenvectors and eigenvalues of C respectively. We then consider the best approximation problem for the IEPs that are solvable. More precisely, given an arbitrary matrix Bin $\mathbb{R}^{n \times n}$, we find the matrix C which is the solution to the IEP and is closest to B in the Frobenius norm. We show that the best approximation is unique and derive an expression for it.

1 Introduction

Let J_n be the *n*-by-*n* anti-identity matrix, i.e, J_n has 1 on the anti-diagonal and zeros elsewhere. An *n*-by-*n* matrix *C* is said to be *centrosymmetric* (or *persymmetric*) if $C = J_n C J_n$, and it is called *centroskew* (or *skew-centrosymmetric*) if $C = -J_n C J_n$. The centrosymmetric and centroskew matrices play an important role in many areas [7, 16] such as signal processing [8, 11], the numerical solution of differential equations [2], and Markov processes [17]. In this paper, we consider two problems related to centrosymmetric and centroskew matrices. Both problems are on numerical and approximate computing but here we solve them algebraically, based on some explicit expressions for the solutions of overdetermined linear systems of equations. The first problem is an inverse eigenproblem. There are many applications of structured inverse eigenproblems, see for instance the expository paper [5]. In particular, the inverse eigenproblem for Toeplitz matrices (a special case of centrosymmetric matrices) arises in trigonometric moment problem [10] and signal processing [9]. The inverse eigenproblem for centrosymmetric Jacobi matrices also comes from inverse Sturm-Liouville problem [19, p.70]. There are also different types of inverse eigenproblem, for instances multiplicative type and additive type [19, Chapter 4]. Here we consider the following type of inverse eigenproblem which appeared in the design of Hopfield neural networks [4, 13].

Problem I. Given $X = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m]$ in $\mathbb{C}^{n \times m}$ and $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_m)$ in $\mathbb{C}^{m \times m}$, find a centrosymmetric or centroskew matrix C in $\mathbb{R}^{n \times n}$ such that $CX = X\Lambda$.

The second problem we consider in this paper is the problem of best approximation:

Problem II. Let \mathcal{L}_S be the solution set of Problem I. Given a matrix $B \in \mathbb{R}^{n \times n}$,
find $C^* \in \mathcal{L}_S$ such that

$$||B - C^*|| = \min_{C \in \mathcal{L}_S} ||B - C||,$$

where $\|\cdot\|$ is the Frobenius norm.

The best approximation problem occurs frequently in experimental design, see for instance [14, p.123]. Here the matrix B may be a matrix obtained from experiments, but it may not satisfy the structural requirement (centrosymmetric or centroskew) and/or spectral requirement (having eigenpairs X and Λ). The best estimate C^* is the matrix that satisfies both requirements and is the best approximation of B in the Frobenius norm. In addition, because there are fast algorithms for solving various kinds of centrosymmetric and centroskew matrices [12], the best approximate C^* of B can also be used as a preconditioner in the preconditioned conjugate gradient method for solving linear systems with coefficient matrix B, see for instance [1].

Problems I and II have been solved for different classes of structured matrices, see for instance [18, 20]. In this paper, we extend the results in [18, 20] to the classes of centrosymmetric and centroskew matrices. We first give a solvability condition for Problem I and also the form of its general solution. Then in the case when Problem I is solvable, we show that Problem II has a unique solution and we give a formula for the minimizer C^* .

The paper is organized as follows: In §2 we first characterize the class of centrosymmetric matrices and give the solvability condition of Problem I over

this class of matrices. In §3, we derive a formula for the best approximation of Problem II, give the algorithm for finding the minimizer, and study the stability of the problem. In §4 we give an example to illustrate the theory. In the last section, we extend the results in §§2–3 to centroskew matrices.

2 Solvability Condition for Problem I

We first characterize the set of all centrosymmetric matrices. For all positive integers k, let

$$K_{2k} = \frac{1}{\sqrt{2}} \begin{bmatrix} I_k & I_k \\ J_k & -J_k \end{bmatrix} \text{ and } K_{2k+1} = \frac{1}{\sqrt{2}} \begin{bmatrix} I_k & \mathbf{0} & I_k \\ \mathbf{0} & \sqrt{2} & \mathbf{0} \\ J_k & \mathbf{0} & -J_k \end{bmatrix}$$

Clearly K_n is orthogonal for all n. The matrix K_n plays an important role in analyzing the properties of centrosymmetric matrices, see for example [6]. In particular, we have the following splitting of centrosymmetric matrices into smaller submatrices using K_n .

Lemma 1 [6] Let C_n be the set of all centrosymmetric matrices in $\mathbb{R}^{n \times n}$. We have

$$\mathcal{C}_{2k} = \left\{ \begin{bmatrix} E & FJ_k \\ J_kF & J_kEJ_k \end{bmatrix} \mid E, F \in \mathbb{R}^{k \times k} \right\},$$
$$\mathcal{C}_{2k+1} = \left\{ \begin{bmatrix} E & \mathbf{a} & FJ_k \\ \mathbf{b}^T & c & \mathbf{b}^TJ_k \\ J_kF & J_k\mathbf{a} & J_kEJ_k \end{bmatrix} \mid E, F \in \mathbb{R}^{k \times k}, \mathbf{a}, \mathbf{b} \in \mathbb{R}^k, c \in \mathbb{R} \right\}$$

Moreover, for all n = 2k and 2k + 1, we have

$$\mathcal{C}_n = \left\{ K_n \left[\begin{array}{cc} G_1 & 0 \\ 0 & G_2 \end{array} \right] K_n^T \mid G_1 \in \mathbb{R}^{(n-k) \times (n-k)}, G_2 \in \mathbb{R}^{k \times k} \right\}.$$
(1)

Before we come to Problem I, we first note that we can assume without loss of generality that X and Λ are real matrices. In fact, since $C_n \subset \mathbb{R}^{n \times n}$, the complex eigenvectors and eigenvalues of any $C \in C_n$ will appear in complex conjugate pairs. If $\alpha \pm \beta \sqrt{-1}$ and $\mathbf{x} \pm \sqrt{-1}\mathbf{y}$ are one of its eigenpair, then we have $C\mathbf{x} = \alpha \mathbf{x} - \beta \mathbf{y}$ and $C\mathbf{y} = \alpha \mathbf{y} + \beta \mathbf{x}$, i.e.

$$C[\mathbf{x}, \mathbf{y}] = [\mathbf{x}, \mathbf{y}] \begin{bmatrix} \alpha & \beta \\ -\beta & \alpha \end{bmatrix}.$$

Hence we can assume without loss of generality that $X \in \mathbb{R}^{n \times m}$ and

$$\Lambda = \operatorname{diag}(\Phi_1, \Phi_2, \dots, \Phi_l, \gamma_1, \dots, \gamma_{m-2l}) \in \mathbb{R}^{m \times m},$$
where $\Phi_i = \begin{bmatrix} \alpha_i & \beta_i \\ -\beta_i & \alpha_i \end{bmatrix}$ with α_i, β_i and γ_i in \mathbb{R} .
$$(2)$$

Next, we investigate the solvability of Problem I. We need the following lemma

where U^+ denotes the Moore-Penrose pseudo-inverse of U.

Lemma 2 [15, Lemma 1.3] Let $U, V \in \mathbb{R}^{n \times m}$ be given. Then YU = V is solvable if and only if $VU^+U = V$. In this case the general solution is

$$Y = VU^+ + Z(I - UU^+),$$

where $Z \in \mathbb{R}^{n \times n}$ is arbitrary.

In the remaining part of the paper, we will only give the theorems and the proofs for even n. The case where n is odd can be proved similarly. Thus we let n = 2k. Centrosymmetric and Centroskew Matrices

Theorem 1 Given $X \in \mathbb{R}^{n \times m}$ and Λ as in (2), let

$$K_n^T X = \begin{bmatrix} \tilde{X}_1 \\ \tilde{X}_2 \end{bmatrix},\tag{3}$$

where $\tilde{X}_2 \in \mathbb{R}^{k \times m}$. Then there exists a matrix $C \in \mathcal{C}_n$ such that $CX = X\Lambda$ if and only if

$$\tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_1 \Lambda \quad \text{and} \quad \tilde{X}_2 \Lambda \tilde{X}_2^+ \tilde{X}_2 = \tilde{X}_2 \Lambda.$$
(4)

In this case, the general solution to $CX = X\Lambda$ is given by

$$C_{s} = C_{0} + K_{n} \begin{bmatrix} Z_{1}(I_{n-k} - \tilde{X}_{1}\tilde{X}_{1}^{+}) & 0\\ 0 & Z_{2}(I_{k} - \tilde{X}_{2}\tilde{X}_{2}^{+}) \end{bmatrix} K_{n}^{T},$$
(5)

where $Z_1 \in \mathbb{R}^{(n-k) \times (n-k)}$ and $Z_2 \in \mathbb{R}^{k \times k}$ are both arbitrary, and

$$C_0 = K_n \begin{bmatrix} \tilde{X}_1 \Lambda \tilde{X}_1^+ & 0\\ 0 & \tilde{X}_2 \Lambda \tilde{X}_2^+ \end{bmatrix} K_n^T.$$
(6)

Proof: From (1), $C \in C_n$ is a solution to Problem I if and only if there exist $G_1 \in \mathbb{R}^{(n-k) \times (n-k)}$ and $G_2 \in \mathbb{R}^{k \times k}$ such that

$$C = K_n \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \end{bmatrix} K_n^T$$
(7)

and

$$\begin{pmatrix} K_n \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \end{bmatrix} K_n^T \end{pmatrix} X = X\Lambda.$$
(8)

Using (3), (8) is equivalent to

$$G_1 \tilde{X}_1 = \tilde{X}_1 \Lambda$$
 and $G_2 \tilde{X}_2 = \tilde{X}_2 \Lambda$. (9)

According to Lemma 2, equations (9) have solutions if and only if equations (4) hold. Moreover in this case, the general solution of (9) is given by

$$G_1 = \tilde{X}_1 \Lambda \tilde{X}_1^+ + Z_1 (I_{n-k} - \tilde{X}_1 \tilde{X}_1^+), \qquad (10)$$

$$G_2 = \tilde{X}_2 \Lambda \tilde{X}_2^+ + Z_2 (I_k - \tilde{X}_2 \tilde{X}_2^+), \qquad (11)$$

where $Z_1 \in \mathbb{R}^{(n-k)\times(n-k)}$ and $Z_2 \in \mathbb{R}^{k\times k}$ are both arbitrary. Putting (10) and (11) into (7), we get (5).

3 The Minimizer of Problem II

Let \mathcal{C}_n^S be the solution set of Problem I over \mathcal{C}_n . In this section, we solve Problem II over \mathcal{C}_n^S when \mathcal{C}_n^S is nonempty.

Theorem 2 Given $X \in \mathbb{R}^{n \times m}$ and Λ as in (2), let the solution set \mathcal{C}_n^S of Problem I be nonempty. Then for any $B \in \mathbb{R}^{n \times n}$, the problem $\min_{C \in \mathcal{C}_n^S} ||B - C||$ has a unique solution C^* given by

$$C^* = C_0 + K_n \begin{bmatrix} \tilde{B}_{11}(I_{n-k} - \tilde{X}_1 \tilde{X}_1^+) & 0\\ 0 & \tilde{B}_{22}(I_k - \tilde{X}_2 \tilde{X}_2^+) \end{bmatrix} K_n^T.$$
(12)

Here \tilde{X}_1 , \tilde{X}_2 , and C_0 are given in (3) and (6), and \tilde{B}_{11} and \tilde{B}_{22} are obtained by partitioning $K_n^T B K_n$ as

$$K_n^T B K_n = \begin{bmatrix} \tilde{B}_{11} & \tilde{B}_{12} \\ \tilde{B}_{21} & \tilde{B}_{22} \end{bmatrix},$$
(13)

where $\tilde{B}_{22} \in \mathbb{R}^{k \times k}$.

Proof: When C_n^S is nonempty, it is easy to verify from (5) that C_n^S is a closed convex set. Since $\mathbb{R}^{n \times n}$ is a uniformly convex Banach space under the Frobenius

norm, there exists a unique solution for Problem II [3, p. 22]. Moreover, because the Frobenius norm is unitary invariant, Problem II is equivalent to

$$\min_{C \in \mathcal{C}_n^S} \|K_n^T B K - K_n^T C K\|^2.$$
(14)

By (5), we have

$$\|K_n^T B K - K_n^T C K\|^2 = \left\| \begin{bmatrix} \tilde{B}_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+ & \tilde{B}_{12} \\ \tilde{B}_{21} & \tilde{B}_{22} - \tilde{X}_2 \Lambda \tilde{X}_2^+ \end{bmatrix} - \begin{bmatrix} Z_1 P & 0 \\ 0 & Z_2 Q \end{bmatrix} \right\|^2,$$

where

$$P = I_{n-k} - \tilde{X}_1 \tilde{X}_1^+$$
 and $Q = I_k - \tilde{X}_2 \tilde{X}_2^+$. (15)

Thus (14) is equivalent to

$$\min_{Z_1 \in \mathbb{R}^{(n-k) \times (n-k)}} \|\tilde{B}_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+ - Z_1 P\|^2 + \min_{Z_2 \in \mathbb{R}^{k \times k}} \|\tilde{B}_{22} - \tilde{X}_2 \Lambda \tilde{X}_2^+ - Z_2 Q\|^2$$

Clearly, the solution is given by Z_1 and Z_2 such that

$$Z_1 P = \tilde{B}_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+ \quad \text{and} \quad Z_2 Q = \tilde{B}_{22} - \tilde{X}_2 \Lambda \tilde{X}_2^+.$$

Notice that by (15), P and Q are projection matrices, i.e. $P^2 = P$ and $Q^2 = Q$. Therefore $Z_1P = (\tilde{B}_{11} - \tilde{X}_1\Lambda\tilde{X}_1^+)P$ and $Z_2Q = (\tilde{B}_{22} - \tilde{X}_2\Lambda\tilde{X}_2^+)Q$. Notice further that because $\tilde{X}_1^+\tilde{X}_1\tilde{X}_1^+ = \tilde{X}_1^+$, we have

$$(\tilde{B}_{11} - \tilde{X}_1 \Lambda \tilde{X}_1^+) P = \tilde{B}_{11} - \tilde{B}_{11} \tilde{X}_1 \tilde{X}_1^+ - \tilde{X}_1 \Lambda \tilde{X}_1^+ + \tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 \tilde{X}_1^+$$

= $\tilde{B}_{11} - \tilde{B}_{11} \tilde{X}_1 \tilde{X}_1^+ = \tilde{B}_{11} P.$

Similarly, $Z_2Q = (\tilde{B}_{22} - \tilde{X}_2\Lambda\tilde{X}_2^+)Q = \tilde{B}_{22}Q$. Hence the unique solution for Problem II is given by (12).

Based on Theorem 2, we give the following algorithm for solving Problem II for n = 2k.

ALGORITHM I

- (a) Compute \tilde{X}_1 and \tilde{X}_2 by (3) and then compute \tilde{X}_1^+ and \tilde{X}_2^+ .
- (b) If $\tilde{X}_1 \Lambda \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_1 \Lambda$ and $\tilde{X}_2 \Lambda \tilde{X}_2^+ \tilde{X}_2 = \tilde{X}_2 \Lambda$, then the solution set \mathcal{C}_n^S to Problem I is nonempty and we continue. Otherwise we stop.
- (c) Partition $K_n^T B K_n$ as in (13) to get \tilde{B}_{11} and \tilde{B}_{22} .
- (d) Compute

$$W_{1} = \tilde{X}_{1}\Lambda\tilde{X}_{1}^{+} + \tilde{B}_{11} - \tilde{B}_{11}\tilde{X}_{1}\tilde{X}_{1}^{+}$$
$$W_{2} = X_{2}\Lambda X_{2}^{+} + \tilde{B}_{22} - \tilde{B}_{22}\tilde{X}_{2}\tilde{X}_{2}^{+}$$
$$(e) \text{ Then } C^{*} = K_{n} \begin{bmatrix} W_{1} & 0 \\ 0 & W_{2} \end{bmatrix} K_{n}^{T}.$$

Next we consider the computational complexity of our algorithm. For Step (a), since K_n has only 2 nonzero entries per row, it requires O(nm) operations to compute \tilde{X}_1 and \tilde{X}_2 . Then using singular value decomposition to compute \tilde{X}_1^+ and \tilde{X}_2^+ requires $O(n^2m + m^3)$ operations. Step (b) obviously requires $O(n^2m)$ operations. For Step (c), because of the sparsity of K_n , the operations required is $O(n^2)$ only. For Step (d), if we compute $\tilde{B}_{ii}\tilde{X}_i\tilde{X}_i^+$ as $[(\tilde{B}_{ii}\tilde{X}_i)\tilde{X}_i^+]$, then the cost will only be of $O(n^2m)$ operations. Finally, because of the sparsity of K_n again, Step (e) requires $O(n^2)$ operations. Thus the total complexity of the algorithm is $O(n^2m + m^3)$. We remark that in practice, $m \ll n$.

Before we end this section, we give a stability analysis for Problem II, that is, we study how the solution of Problem II is affected by a small perturbation of B. We have the following result.

Corollary 1 Given $B^{(i)} \in \mathbb{R}^{n \times n}$, i = 1, 2. Let $C^{*(i)} = \arg\min_{C \in \mathcal{C}_n^S} ||B^{(i)} - C||$ for i = 1, 2. Then there exists a constant α independent of $B^{(i)}$, i = 1, 2, such that

$$\|C^{*(2)} - C^{*(1)}\| \le \alpha \|B^{(2)} - B^{(1)}\|.$$
(16)

Proof: By Theorem 2, $C^{*(i)}$ is given by

$$C^{*(i)} = C_0 + K_n \begin{bmatrix} \tilde{B}_{11}^{(i)} P & 0\\ 0 & \tilde{B}_{22}^{(i)} Q \end{bmatrix} K_n^T, \quad i = 1, 2,$$

where $\tilde{B}_{22}^{(i)}$ are the blocks of $K_n^T B^{(i)} K_n$ as defined in (13), and P and Q are given in (15). Thus we have

$$\begin{split} \|C^{*(2)} - C^{*(1)}\| &= \left\| K_n \begin{bmatrix} \left(\tilde{B}_{11}^{(2)} - \tilde{B}_{11}^{(1)} \right) P & 0 \\ 0 & \left(\tilde{B}_{22}^{(2)} - \tilde{B}_{22}^{(1)} \right) Q \end{bmatrix} K_n^T \right\| \\ &\leq \left\| \begin{bmatrix} \tilde{B}_{11}^{(2)} - \tilde{B}_{11}^{(1)} & 0 \\ 0 & \tilde{B}_{22}^{(2)} - \tilde{B}_{22}^{(1)} \end{bmatrix} \right\| \left\| \begin{bmatrix} P & 0 \\ 0 & Q \end{bmatrix} \right\| \\ &\leq \left\| K_n^T \left(B^{(2)} - B^{(1)} \right) K_n \right\| \left\| \begin{bmatrix} P & 0 \\ 0 & Q \end{bmatrix} \right\| \\ &\leq \alpha \left\| B^{(2)} - B^{(1)} \right\|, \end{split}$$

where $\alpha = ||P|| + ||Q||$. Thus (16) holds.

4 Demonstration by an Example

Let us first compute the input matrices X and Λ for which Problem I has a solution. We start by choosing a random matrix \hat{C} in \mathcal{C}_n :

$$\hat{C} = \begin{bmatrix} 0.1749 & 0.0325 & -0.2046 & 0.0932 & 0.0315 \\ 0.0133 & -0.0794 & -0.0644 & 0.1165 & -0.0527 \\ 0.1741 & 0.0487 & 0.1049 & 0.0487 & 0.1741 \\ -0.0527 & 0.1165 & -0.0644 & -0.0794 & 0.0133 \\ 0.0315 & 0.0932 & -0.2046 & 0.0325 & 0.1749 \end{bmatrix} \in \mathbb{C}_5.$$

Then we compute its eigenpairs. The eigenvalues of \hat{C} are $0.1590 \pm 0.2841\sqrt{-1}$, -0.1836, 0.1312, and 0.0304. Let $\mathbf{x}_1 \pm \sqrt{-1}\mathbf{x}_2$, \mathbf{x}_3 , \mathbf{x}_4 , and \mathbf{x}_5 be the corresponding eigenvectors. Then we take

$$X = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5] = \begin{bmatrix} 0.4815 & 0.2256 & -0.2455 & -0.7071 & -0.1313 \\ 0.0118 & 0.1700 & 0.7071 & -0.1427 & -0.7071 \\ 0.4322 & -0.5120 & 0.2235 & 0 & 0 \\ 0.0118 & 0.1700 & 0.7071 & 0.1427 & 0.7071 \\ 0.4815 & 0.2256 & -0.2455 & 0.7071 & 0.1313 \end{bmatrix}$$

and

$$\Lambda = \begin{bmatrix} 0.1590 & 0.2841 & 0 & 0 & 0 \\ -0.2841 & 0.1590 & 0 & 0 & 0 \\ 0 & 0 & 0.0304 & 0 & 0 \\ 0 & 0 & 0 & 0.1312 & 0 \\ 0 & 0 & 0 & 0 & -0.1836 \end{bmatrix}$$

Given this X and A, clearly we have a solution to Problem I, namely \hat{C} . Thus \mathcal{C}_5^S is nonempty. Next we perturb \hat{C} by a random matrix to obtain a matrix $B(\epsilon) \notin \mathcal{C}_5$:

$$B(\epsilon) = \hat{C} + \epsilon \cdot \begin{bmatrix} 1.4886 & -0.9173 & 1.2688 & -0.1869 & -1.0830 \\ 1.2705 & -1.1061 & -0.7836 & 1.0132 & 1.0354 \\ -1.8561 & 0.8106 & 0.2133 & 0.2484 & 1.5854 \\ 2.1343 & 0.6985 & 0.7879 & 0.0596 & 0.9157 \\ 1.4358 & -0.4016 & 0.8967 & 1.3766 & -0.5565 \end{bmatrix}.$$

Then we can apply our algorithm in §3 to obtain $C^*(\epsilon)$ corresponding to $B(\epsilon)$. In Figure 1, we plot the following two quantities for ϵ between 10^{-10} to 10^{10} : $\log_{10} \|B(\epsilon) - C^*(\epsilon)\|$ (marked by "*") and $\log_{10} \|\hat{C} - C^*(\epsilon)\|$ (marked by "+"). We can see that as ϵ goes to zero, $C^*(\epsilon)$ approaches $B(\epsilon)$ as expected. Also when $\epsilon \leq 10^{-1}$, $C^*(\epsilon) = \hat{C}$ up to the machine precision (we use MATLAB which has machine precision around 10^{-16}).



Figure 1: $\log_{10} \|B(\epsilon) - C^*(\epsilon)\|$ ("*") and $\log_{10} \|\hat{C} - C^*(\epsilon)\|$ ("+") versus $\log_{10} \epsilon$.

5 Extension to the Set of Centroskew Matrices

In this section, we extend our results in §§2–3 to centroskew matrices, i.e. matrices S such that $S = -J_n S J_n$. The results and the proofs are similar to the centrosymmetric case, and we only list the results for the case when n is even and omit the proofs. Let n = 2k. Considering Problem I for S_n , we have the following theorem.

Theorem 3 Given $X \in \mathbb{R}^{n \times m}$ and Λ as in (2), let \tilde{X}_1 and \tilde{X}_2 be as defined in (3). Then there exists $S \in S_n$ such that $SX = X\Lambda$ if and only if

$$\tilde{X}_1 \Lambda \tilde{X}_2^+ \tilde{X}_2 = \tilde{X}_1 \Lambda$$
 and $\tilde{X}_2 \Lambda \tilde{X}_1^+ \tilde{X}_1 = \tilde{X}_2 \Lambda$.

In this case, the general solution to $SX = X\Lambda$ is given by

$$S_{s} = S_{0} + K_{n} \begin{bmatrix} 0 & Z_{1}(I_{k} - \tilde{X}_{2}\tilde{X}_{2}^{+}) \\ Z_{2}(I_{k} - \tilde{X}_{1}\tilde{X}_{1}^{+}) & 0 \end{bmatrix} K_{n}^{T},$$

where $Z_1 \in \mathbb{R}^{k \times k}$ and $Z_2 \in \mathbb{R}^{k \times k}$ are both arbitrary, and

$$S_0 = K_n \begin{bmatrix} 0 & \tilde{X}_1 \Lambda \tilde{X}_2^+ \\ \tilde{X}_2 \Lambda \tilde{X}_1^+ & 0 \end{bmatrix} K_n^T.$$
(17)

For Problem II over the solution set S_n^S of Problem I for S_n , we have the following result.

Theorem 4 Given $X \in \mathbb{R}^{n \times m}$ and Λ as in (2), let the solution set S_n^S of Problem I be nonempty. Then for any $B \in \mathbb{R}^{n \times n}$, the problem $\min_{S \in S_n^S} ||B - S||$ has a unique solution S^* given by

$$S^* = S_0 + K_n \left[\begin{array}{cc} 0 & \tilde{B}_{12}(I_k - \tilde{X}_2 \tilde{X}_2^+) \\ \tilde{B}_{21}(I_{n-k} - \tilde{X}_1 \tilde{X}_1^+) & 0 \end{array} \right] K_n^T$$

Here \tilde{X}_1 , \tilde{X}_2 , \tilde{B}_{12} , \tilde{B}_{21} , and S_0 are given in (3), (13), and (17). Moreover S^* is a continuous function of B.

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