MATHEMATICAL ENGINEERING
TECHNICAL REPORTS

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METR 2017–17 August 2017

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August 2017

Abstract

In 2017, for inverse symmetric eigenvalue problems, a new quadratically convergent algorithm has been derived from simple matrix equations. Although this algorithm has some nice features compared with the other quadratically convergent methods, it is not applied to multiple eigenvalues. In this paper, we improve this algorithm with the aid of an optimization problem for the eigenvectors associated with multiple eigenvalues. The proposed algorithm is adapted to an arbitrary set of given eigenvalues. The main contribution is our convergence theorem formulated in a different manner from previous work for the existing quadratically convergent methods. Our theorem ensures the quadratic convergence in a neighborhood of the solutions that satisfy a mild condition.

1 Introduction

Let $A_0, A_1, \ldots, A_n$ be real symmetric $n \times n$ matrices and

$$\lambda_1^* \leq \lambda_2^* \leq \cdots \leq \lambda_n^*$$

be real numbers. In addition, let $\boldsymbol{c} = [c_1, \ldots, c_n]^{\mathrm{T}} \in \mathbb{R}^n$ and

$$\Lambda^* = \mathrm{diag}(\lambda_1^*, \ldots, \lambda_n^*).$$

Define

$$A(\boldsymbol{c}) := A_0 + c_1 A_1 + \cdots + c_n A_n, \tag{1}$$

and denote its eigenvalues by $\lambda_1(\boldsymbol{c}) \leq \lambda_2(\boldsymbol{c}) \leq \cdots \leq \lambda_n(\boldsymbol{c})$ in the ascending order. A typical inverse eigenvalue problem is to find $\boldsymbol{c}^* \in \mathbb{R}^n$ such that

$\lambda_i(\boldsymbol{c}^*) = \lambda_i^*$ for all $1 \le i \le n$. Such inverse eigenvalue problems often arise in a variety of applications, e.g., inverse Sturm–Liouville problems, inverse vibration problems, and nuclear spectroscopy [6, 7, 8, 14]. In this study, we focus on numerical algorithms for solving the above inverse eigenvalue problems. Throughout the paper, I is an identity matrix, and O is a zero matrix. For any matrix, let $\|\cdot\|$ denote the spectral norm and $[\cdot]_{ij}$ denote the (i, j) elements for $1 \le i, j \le n$.

There are various quadratically convergent methods for solving the above problems. A typical method is the following Newton's method. Define $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$ by $\boldsymbol{f}(\boldsymbol{c}) = [\lambda_1(\boldsymbol{c}), \ldots, \lambda_n(\boldsymbol{c})]$, where $\lambda_1(\boldsymbol{c}) \le \cdots \le \lambda_n(\boldsymbol{c})$ are eigenvalues of $A(\boldsymbol{c})$. The Newton's method computes $\boldsymbol{c}^*$ such that $\boldsymbol{f}(\boldsymbol{c}^*) = 0$, where the convergence rate is quadratic [14, Method I]. Since this approach is straightforward, it can be extended to more general inverse eigenvalue problems [11, 12]. However, the Newton's method for the above nonlinear equation $\boldsymbol{f}(\boldsymbol{c}) = 0$ requires an eigenvalue decomposition in each iteration. Hence, a Newton-like method was derived from an approximation of the eigenvalue decomposition [14, Method II]; see [3, 4, 18] for the details of the algorithm developments and its convergence theory. Moreover, there is a different approach with the use of matrix exponentials and Cayley transforms [14, Method III]. This algorithm is now called the Cayley transform method, which is also well studied [2, 5, 17, 19]. Furthermore, on the basis of a different formulation: $\det(A(\boldsymbol{c}^*) - \lambda_i^* I) = 0$ for all $i = 1, \ldots, n$, another quadratically convergent method is derived as in [14, Method IV]. Some quadratically convergent methods have been proposed for more general problems from the above formulation with some matrix factorizations in recent studies [9, 10, 13]. However, according to the discussion in [14, §2], the method as in [14, Method IV] almost always requires more iterations than the Newton's method for $\boldsymbol{f}(\boldsymbol{c}) = 0$ as in [14, Method I] in the numerical experiments.

In this paper, we focus on a latest iterative algorithm in [1], which is summarized as follows. Let $\boldsymbol{x}_i^*$ for $i = 1, \ldots, n$ denote normalized eigenvectors corresponding to the eigenvalues λ_i^* for $i = 1, \ldots, n$. In addition, let $X^* := [\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*] \in \mathbb{R}^{n\times n}$, which is an orthogonal matrix. For computed matrices $X^{(k)} \in \mathbb{R}^{n\times n}$ $(k = 0, 1, \ldots)$ in the iterative process, define $E^{(k)} \in \mathbb{R}^{n\times n}$ $(k = 0, 1, \ldots)$ such that $X^{(k)} = X^*(I + E^{(k)})$ based on the orthonormal set of the eigenvectors $\{\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*\}$. Then we compute $\widetilde{E}^{(k)}$ approximating $E^{(k)}$ from the following relations:

$$\begin{cases} X^{*\mathrm{T}} X^* = I, \\ X^{*\mathrm{T}} A(\boldsymbol{c}^*) X^* = \Lambda^*. \end{cases} \tag{2}$$

After computing $\widetilde{E}^{(k)}$, we can update $X^{(k+1)} := X^{(k)}(I - \widetilde{E}^{(k)})$, where $I - \widetilde{E}^{(k)}$ is the first order approximation of $(I + \widetilde{E}^{(k)})^{-1}$ using the Neumann series. Under some conditions, $E^{(k)} \to O$ and $X^{(k)} \to X^*$ as $k \to \infty$ are proved, where the convergence rates are quadratic.

Although this algorithm has some nice features compared with the other quadratically convergent methods, it is not applied to multiple eigenvalues. With such a background, our aim is to modify this algorithm to solve the problems with multiple eigenvalues. Our approach is based on an optimization problem, namely the orthogonal Procrustes problem [15, §6.4.1]. As a result, the columns of $X^{(k)}$ $(k = 0, 1, \dots)$ associated with multiple eigenvalues are computed with the aid of the polar decomposition, different from the usual way explicitly computing the QR factorization as in [14, 18, 19]. Such an idea using the polar decomposition is also found in [16] that presents an efficient iterative refinement algorithms for symmetric eigenvalue problems. In this sense, our approach to multiple eigenvalues is straightforward. Noting the above algorithm design, we provide convergence theory to ensure the quadratic convergence under a technical assumption. The main contribution is the convergence theorem derived from Lemmas 4 and 5 newly shown in this paper. It is worth noting that our convergence theorem is a different formulation from the previous work for the existing quadratically convergent methods.

This paper is organized as follows. In Section 2, we derive a new algorithm applied to multiple eigenvalues, modifying the basic algorithm presented in [1]. In Section 3, we prove quadratic convergence of the proposed algorithm. The strength of our convergence analysis is described in Section 4. In Section 5, we report a numerical result to illustrate our convergence theory. Concluding remarks are given in Section 6.

2 Proposed algorithm

In this section, we derive a new algorithm based on the relations in (2). Before that, we briefly review a basic algorithm presented in [1] for the situation where all prescribed eigenvalues are distinct, i.e., $\lambda_1^* < \cdots < \lambda_n^*$. As in the previous section, for a given $X^{(k)} \in \mathbb{R}^{n\times n}$, define $E^{(k)} \in \mathbb{R}^{n\times n}$ such that

$$X^{(k)} = X^*(I + E^{(k)}), \tag{3}$$

where $X^{(k)}$ is assumed to be sufficiently close to X^*. First, using $X^{*\mathrm{T}}X^* = I$ in (2), we have

$$I + E^{(k)} + E^{(k)\mathrm{T}} + \Delta_1^{(k)} = X^{(k)\mathrm{T}}X^{(k)}, \quad \Delta_1^{(k)} := E^{(k)\mathrm{T}}E^{(k)}. \tag{4}$$

Since we assume $\|E^{(k)}\|$ is sufficiently small, omitting the quadratic term $\|\Delta_1^{(k)}\| \le \|E^{(k)}\|^2$, we obtain the following matrix equation for $\widetilde{E}^{(k)}$:

$$\widetilde{E}^{(k)} + \widetilde{E}^{(k)\mathrm{T}} = X^{(k)\mathrm{T}}X^{(k)} - I. \tag{5}$$

Next, noting $X^{*\mathrm{T}}A(\boldsymbol{c}^*)X^* = \Lambda^*$ in (2), we have

$$\Lambda^* + \Lambda^* E^{(k)} + E^{(k)\mathrm{T}}\Lambda^* + \Delta_2^{(k)} = X^{(k)\mathrm{T}}A(\boldsymbol{c}^*)X^{(k)}, \quad \Delta_2^{(k)} := E^{(k)\mathrm{T}}\Lambda^* E^{(k)}. \tag{6}$$

As in (5), omitting $\Delta_2^{(k)}$, we have the following equation for $\widetilde{E}^{(k)}$ and $\boldsymbol{c}^{(k+1)}$:

$$\Lambda^* + \Lambda^* \widetilde{E}^{(k)} + \widetilde{E}^{(k)\mathrm{T}}\Lambda^* = X^{(k)\mathrm{T}}A(\boldsymbol{c}^{(k+1)})X^{(k)}. \tag{7}$$

Combining (5) and (7), we obtain the following equations:

$$\begin{cases} I + \widetilde{E}^{(k)} + \widetilde{E}^{(k)\mathrm{T}} = X^{(k)\mathrm{T}}X^{(k)}, \\ \Lambda^* + \Lambda^* \widetilde{E}^{(k)} + \widetilde{E}^{(k)\mathrm{T}}\Lambda^* = X^{(k)\mathrm{T}}A(\boldsymbol{c}^{(k+1)})X^{(k)}, \end{cases} \tag{8}$$

where the elements of $\widetilde{E}^{(k)}$ and $\boldsymbol{c}^{(k+1)}$ are unknown variables. In (8), $\widetilde{E}^{(k)}$ and $\boldsymbol{c}^{(k+1)}$ can be easily obtained as shown in [1].

However, if Λ^* has multiple eigenvalues, the matrix equations in (8) have no solutions in general, and hence some modifications are required. For simplicity, we assume that the first p eigenvalues are multiple, i.e.,

$$\lambda_1^* = \cdots = \lambda_p^* < \lambda_{p+1}^* < \cdots < \lambda_n^*$$

in the same manner as [14, 17, 18, 19]. It is easy to generalize the following discussion to an arbitrary set of prescribed eigenvalues as shown later.

First of all, note that, even if the problem has a locally unique solution $\boldsymbol{c}^*$, the corresponding X^* as in (2) is not unique. In other words, $X_p^* := [\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_p^*]$ associated with the multiple eigenvalues is not unique. More specifically, for any orthogonal matrix $Q \in \mathbb{R}^{p\times p}$, all the columns of X_p^*Q are also eigenvectors. Hence, for a given $X^{(k)}$, let

$$Y^{(k)} := \arg\min_{X^*} \|X^* - X^{(k)}\|_{\mathrm{F}}, \tag{9}$$

where $\|\cdot\|_{\mathrm{F}}$ denotes the Frobenius norm. In addition, define $F^{(k)}$ that satisfies

$$X^{(k)} = Y^{(k)}(I + F^{(k)}). \tag{10}$$

Then, we see

$$\|F^{(k)}\|_{\mathrm{F}} = \|X^{(k)} - Y^{(k)}\|_{\mathrm{F}} = \min_{X^*} \|X^* - X^{(k)}\|_{\mathrm{F}} \tag{11}$$

from easy calculations.

For a given $X^{(k)}$, the above $F^{(k)}$ is locally unique, and the leading principal $p\times p$ submatrix of $F^{(k)}$ is symmetric matrix. Such a feature is relevant to the orthogonal Procrustes problem [15, §6.4.1]. In other words, for fixed X_p^* and $X_p^{(k)}$, we consider an optimization problem

$$\min_{Q^{(k)\mathrm{T}}Q^{(k)}=I} \|X_p^* Q^{(k)} - X_p^{(k)}\|_{\mathrm{F}}, \tag{12}$$

relevant to (9). We can obtain the optimal $Q^{(k)}$ using the polar decomposition

$$Q^{(k)}T^{(k)} := X_p^{*\mathrm{T}} X_p^{(k)}, \tag{13}$$

where $Q^{(k)}$ is an orthogonal matrix, and $T^{(k)}$ is a positive semi-definite matrix, as shown in [15, §6.4.1]. Note that $T^{(k)}$ in (13) is independent of the choice of X_p^* because of the uniqueness of the polar decomposition, while the solution $Q^{(k)}$ depends on X_p^*. Therefore, for the solution $Y^{(k)} = [\boldsymbol{y}_1, \dots, \boldsymbol{y}_n]$ in (9), we see

$$\begin{aligned} &Y_p^{(k)} := [\boldsymbol{y}_1, \dots, \boldsymbol{y}_p], \\ &Y_p^{(k)\mathrm{T}} X_p^{(k)} = (X_p^* Q^{(k)})^{\mathrm{T}} X_p^{(k)} = T^{(k)}, \end{aligned}$$

which implies that the leading principal $p \times p$ submatrix of $F^{(k)}$ in (10) is equal to the symmetric matrix $T^{(k)} - I_p$ ($I_p \in \mathbb{R}^{p \times p}$). Note that the above discussion is easily generalized to an arbitrary set of prescribed eigenvalues. In summary, we have the next lemma for any eigenvalue distribution $\lambda_1^* \leq \dots \leq \lambda_n^*$.

Lemma 1. *For any fixed $X^{(k)}$, suppose that $Y^{(k)}$ and $F^{(k)}$ are defined as* (9) *and* (10)*, respectively. Then, $F^{(k)}$ satisfies* (11) *and $[F^{(k)}]_{ij} = [F^{(k)}]_{ji}$ for i, j corresponding to multiple eigenvalues $\lambda_i^* = \lambda_j^*$.*

Our aim is to obtain $\widetilde{F}^{(k)}$ approximating $F^{(k)}$ using the above lemma. To this end, using $Y^{(k)\mathrm{T}} Y^{(k)} = I$ in (2), we have

$$I + F^{(k)} + F^{(k)\mathrm{T}} + \Delta_1^{(k)} = X^{(k)\mathrm{T}} X^{(k)}, \quad \Delta_1^{(k)} := F^{(k)\mathrm{T}} F^{(k)}. \tag{14}$$

Next, noting $Y^{(k)\mathrm{T}} A(\boldsymbol{c}^*) Y^{(k)} = \Lambda^*$ in (2), we have

$$\Lambda^* + \Lambda^* F^{(k)} + F^{(k)\mathrm{T}} \Lambda^* + \Delta_2^{(k)} = X^{(k)\mathrm{T}} A(\boldsymbol{c}^*) X^{(k)}, \quad \Delta_2^{(k)} := F^{(k)\mathrm{T}} \Lambda^* F^{(k)}. \tag{15}$$

Noting the diagonal elements for (14) and (15), we have the following linearized equations:

$$\begin{cases} \left[I + \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}}\right]_{ii} = \left[X^{(k)\mathrm{T}} X^{(k)}\right]_{ii} \\ \left[\Lambda^* + \Lambda^* \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}} \Lambda^*\right]_{ii} = \left[X^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) X^{(k)}\right]_{ii} \end{cases} \tag{16}$$

for $i = 1, \dots, n$. The linearization for the off-diagonal elements is slightly different from the basic version for the situation where the eigenvalues are all distinct. For $i \neq j$ corresponding to $\lambda_i^* = \lambda_j^*$, on the basis of the above symmetry of $F^{(k)}$ in Lemma 1, let

$$\begin{cases} \left[I + \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}}\right]_{ij} = \left[X^{(k)\mathrm{T}} X^{(k)}\right]_{ij} \\ \left[\widetilde{F}^{(k)}\right]_{ij} = \left[\widetilde{F}^{(k)}\right]_{ji} \end{cases}. \tag{17}$$

On the other hand, for $i \neq j$ corresponding to $\lambda_i^* \neq \lambda_j^*$, let

$$\begin{cases} \left[I + \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}}\right]_{ij} = \left[X^{(k)\mathrm{T}} X^{(k)}\right]_{ij} \\ \left[\Lambda^* + \Lambda^* \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}} \Lambda^*\right]_{ij} = \left[X^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) X^{(k)}\right]_{ij} \end{cases} \tag{18}$$

in the same manner as the basic algorithm.

Similarly to the basic algorithm in [1], the above equations can be easily solved as follows. First, noting the first equation in (16), we see

$$[\widetilde{F}^{(k)}]_{ii} = \frac{\boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_i^{(k)} - 1}{2} \quad (1 \leq i \leq n). \tag{19}$$

In addition, for $i \neq j$ corresponding to multiple eigenvalues $\lambda_i^* = \lambda_j^*$,

$$[\widetilde{F}^{(k)}]_{ij} = \frac{\boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_j^{(k)}}{2} \quad (1 \leq i, j \leq n,\ i \neq j,\ \lambda_i^* = \lambda_j^*) \tag{20}$$

from (17).

Next, we compute $\boldsymbol{c}^{(k+1)}$ as follows. For the left hand-side of the second equation in (16), we have

$$\begin{aligned} [\Lambda^* + \Lambda^* \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}} \Lambda^*]_{ii} &= [\Lambda^* (I + \widetilde{F}^{(k)} + \widetilde{F}^{(k)\mathrm{T}})]_{ii} \\ &= \lambda_i^* \boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_i^{(k)} \end{aligned} \tag{21}$$

for $i = 1, \ldots, n$, where the second equality is due to the first equation in (16). Here, letting

$$[J^{(k)}]_{ij} = \boldsymbol{x}_i^{(k)\mathrm{T}} A_j \boldsymbol{x}_i^{(k)} \quad (1 \leq i, j \leq n), \tag{22}$$

we have

$$[X^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) X^{(k)}]_{ii} = [J^{(k)} \boldsymbol{c}^{(k+1)}]_i + \boldsymbol{x}_i^{(k)\mathrm{T}} A_0 \boldsymbol{x}_i^{(k)} \quad (1 \leq i \leq n). \tag{23}$$

Therefore, letting

$$[\boldsymbol{d}^{(k)}]_i = \lambda_i^* \boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_i^{(k)} - \boldsymbol{x}_i^{(k)\mathrm{T}} A_0 \boldsymbol{x}_i^{(k)} \quad (1 \leq i \leq n),$$

we obtain

$$\boldsymbol{c}^{(k+1)} = (J^{(k)})^{-1} \boldsymbol{d}^{(k)} \tag{24}$$

by (16), (21), and (23).

Finally, we compute the off-diagonal parts of $\widetilde{F}^{(k)}$ corresponding to the distinct eigenvalues $\lambda_i^* \neq \lambda_j^*$. Using (24), in each (i, j) element of (18) we see the following 2×2 linear system

$$\begin{cases} [\widetilde{F}^{(k)}]_{ij} + [\widetilde{F}^{(k)}]_{ji} = \boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_j^{(k)} \\ \lambda_i^* [\widetilde{F}^{(k)}]_{ij} + \lambda_j^* [\widetilde{F}^{(k)}]_{ji} = \boldsymbol{x}_i^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) \boldsymbol{x}_j^{(k)} \end{cases} \quad (1 \leq i, j \leq n, \lambda_i^* \neq \lambda_j^*).$$

Therefore, we obtain

$$[\widetilde{F}^{(k)}]_{ij} = \frac{\lambda_j^* \boldsymbol{x}_i^{(k)\mathrm{T}} \boldsymbol{x}_j^{(k)} - \boldsymbol{x}_i^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) \boldsymbol{x}_j^{(k)}}{\lambda_j^* - \lambda_i^*} \quad (1 \le i, j \le n, \lambda_i^* \ne \lambda_j^*). \tag{25}$$

As a result, we can compute the next step

$$X^{(k+1)} = X^{(k)}(I - \widetilde{F}^{(k)}), \tag{26}$$

where $I - \widetilde{F}^{(k)}$ is the first order approximation of $(I + \widetilde{F}^{(k)})^{-1}$ using the Neumann series. In Algorithm 1, we present the proposed algorithm.

Algorithm 1 The proposed algorithm.

Require: $\lambda_1^* \le \cdots \le \lambda_n^*$, $A_0, \ldots, A_n \in \mathbb{R}^{n \times n}$; $X^{(0)} \in \mathbb{R}^{n \times n}$

1: **for** $k = 0, 1, \ldots$ **do**
2: $\quad R^{(k)} = X^{(k)\mathrm{T}} X^{(k)}$
3: $\quad [\widetilde{F}^{(k)}]_{ii} = ([R^{(k)}]_{ii} - 1)/2 \quad (1 \le i \le n)$
4: $\quad [J^{(k)}]_{ij} = \boldsymbol{x}_i^{(k)\mathrm{T}} A_j \boldsymbol{x}_i^{(k)} \quad (1 \le i, j \le n)$
5: $\quad [\boldsymbol{d}^{(k)}]_i = \lambda_i^* [R^{(k)}]_{ii} - \boldsymbol{x}_i^{(k)\mathrm{T}} A_0 \boldsymbol{x}_i^{(k)} \quad (1 \le i \le n)$
6: $\quad \boldsymbol{c}^{(k+1)} = (J^{(k)})^{-1} \boldsymbol{d}^{(k)}$
7: $\quad S^{(k+1)} = X^{(k)\mathrm{T}} A(\boldsymbol{c}^{(k+1)}) X^{(k)}$
8: $\quad$ **if** $\lambda_i^* = \lambda_j^*$ **then**
9: $\quad\quad \widetilde{F}_{ij}^{(k)} = [R^{(k)}]_{ij}/2 \quad (1 \le i, j \le n,\ i \ne j)$
10: $\quad$ **else**
11: $\quad\quad [\widetilde{F}^{(k)}]_{ij} = (\lambda_j^* [R^{(k)}]_{ij} - [S^{(k+1)}]_{ij})/(\lambda_j^* - \lambda_i^*) \quad (1 \le i, j \le n,\ i \ne j)$
12: $\quad$ **end if**
13: $\quad X^{(k+1)} = X^{(k)}(I - \widetilde{F}^{(k)})$
14: **end for**

In 2017, a similar algorithm is proposed in [19], while the proposed algorithm is based on an approximation of the Cayley transform different from Algorithm 1. To clarify it, let us introduce the normalizations of $\boldsymbol{x}_i^{(k+1)}$ $(i = 1, \ldots, n)$ for $X^{(k+1)}$. In other words, if line 13 is replaced with

$$\begin{aligned}
&\widetilde{X}^{(k+1)} (:= [\widetilde{\boldsymbol{x}}_1^{(k+1)}, \ldots, \widetilde{\boldsymbol{x}}_n^{(k+1)}]) = X^{(k)}(I - \widetilde{F}^{(k)}), \\
&\boldsymbol{x}_i^{(k+1)} = \widetilde{\boldsymbol{x}}_i^{(k+1)} / \|\widetilde{\boldsymbol{x}}_i^{(k+1)}\| \quad (i = 1, \ldots, n), \\
&X^{(k+1)} = [\boldsymbol{x}_1^{(k+1)}, \ldots, \boldsymbol{x}_n^{(k+1)}],
\end{aligned}$$

then this variant of Algorithm 1 is equivalent to the algorithm in [19] whenever the prescribed eigenvalues are all distinct. However, if multiple eigenvalues are present, this variant is also different from the algorithm in [19]. More importantly, we can provide a novel convergence theorem based on our algorithm design different from existing formulations in the next section. The strength of our convergence analysis is described in Section 4. In addition, note that the basic idea using the polar decomposition is also found in [16] that presents an efficient iterative refinement algorithms for symmetric eigenvalue problems. In this sense, our approach to multiple eigenvalues is straightforward.

3 Convergence analysis

In this section, we prove quadratic convergence of the proposed algorithm under some assumption that $X^{(k)}$ for some k is sufficiently close to an eigenvector matrix of $A(\boldsymbol{c}^*)$.

In the following, we would like to use the spectral norm as usual, though $Y^{(k)}$ is the optimal matrix in terms of the Frobenius norm as Lemma 1. Obviously,

$$\|Y^{(k)} - X^{(k)}\| \le \|Y^{(k)} - X^{(k)}\|_{\mathrm{F}} \le \|X^* - X^{(k)}\|_{\mathrm{F}} \le \sqrt{n}\|X^* - X^{(k)}\|$$

for any X^*. Thus, letting $\{E^{(k)} \mid X^{(k)} = X^*(I + E^{(k)})\}$, we have

$$\|F^{(k)}\| \le \sqrt{n}\|E^{(k)}\|$$

for any $E^{(k)}$ in terms of the spectral norm. In fact, $\sqrt{n}$ can be replaced with 3 as follows, which is essentially proved in [16, Lemma 4].

Lemma 2. *For a given $X^{(k)} \in \mathbb{R}^{n\times n}$, let $\{X^*\}$ be the set of the $n \times n$ eigenvector matrices for $A(\boldsymbol{c}^*)$ and*

$$\{E^{(k)} \mid X^{(k)} = X^*(I + E^{(k)})\}. \tag{27}$$

In addition, $F^{(k)}$ is defined as in Lemma 1. Then, for any $E^{(k)}$,

$$\|F^{(k)}\| \le 3\|E^{(k)}\|. \tag{28}$$

Proof. For any $E^{(k)}$ in (27), define a block diagonal matrix $E^{(k)}_{\mathrm{diag}}$ such that

$$[E^{(k)}_{\mathrm{diag}}]_{ij} := \begin{cases} [E^{(k)}]_{ij} & (\lambda_i^* = \lambda_j^*) \\ 0 & (\text{otherwise}) \end{cases},$$

related to the block diagonal part of $F^{(k)}$. Here, we consider the polar decomposition

$$I + E^{(k)}_{\mathrm{diag}} =: U^{(k)}H^{(k)}, \tag{29}$$

where $H^{(k)}$ is a symmetric positive definite matrix, and $U^{(k)}$ is an orthogonal matrix. Then, noting

$$X^{(k)} = (X^*U^{(k)})U^{(k)\mathrm{T}}(I + E^{(k)}),$$

we have

$$Y^{(k)} = X^* U^{(k)} \tag{30}$$

from the definition of $Y^{(k)}$ as in Lemma 1, and

$$\begin{aligned} F^{(k)} &= Y^{(k)\mathrm{T}} X^{(k)} - I \\ &= U^{(k)\mathrm{T}} X^{*\mathrm{T}} X^{(k)} - I \\ &= U^{(k)\mathrm{T}} (E^{(k)} + I) - I \\ &= U^{(k)\mathrm{T}} (E^{(k)} - E^{(k)}_{\mathrm{diag}} + U^{(k)} H^{(k)}) - I \\ &= U^{(k)\mathrm{T}} (E^{(k)} - E^{(k)}_{\mathrm{diag}}) + H^{(k)} - I, \end{aligned} \tag{31}$$

where the first, second, third, and fourth equalities are consequences of (10), (30), (27), and (29), respectively. In addition, we see that

$$\|H^{(k)} - I\| \leq \|E^{(k)}_{\mathrm{diag}}\| \tag{32}$$

because all eigenvalues of $H^{(k)}$ range over the interval $[1 - \|E^{(k)}_{\mathrm{diag}}\|, 1 + \|E^{(k)}_{\mathrm{diag}}\|]$ from (29). Moreover, note that

$$\|E^{(k)}_{\mathrm{diag}}\| \leq \|E^{(k)}\|. \tag{33}$$

Therefore, we obtain

$$\|F^{(k)}\| \leq \|U^{(k)\mathrm{T}} (E^{(k)} - E^{(k)}_{\mathrm{diag}})\| + \|H^{(k)} - I\| \leq 3\|E^{(k)}\|$$

from (31), (32), and (33), giving us (28). □

Next, we focus on the relationship between $F^{(k)}$ and $\widetilde{F}^{(k)}$. From (14), (15), (16), (17), and (18), we have

$$\Delta_{\widetilde{F}^{(k)}} := F^{(k)} - \widetilde{F}^{(k)},$$

$$\Delta_{\widetilde{F}^{(k)}} + \Delta_{\widetilde{F}^{(k)}}{}^{\mathrm{T}} + \Delta_1^{(k)} = O, \tag{34}$$

$$\begin{cases} \left[\Delta_{\widetilde{F}^{(k)}}\right]_{ij} = \left[\Delta_{\widetilde{F}^{(k)}}\right]_{ji} & (\text{if } i \neq j \text{ and } \lambda_i^* = \lambda_j^*) \\ \left[\Lambda^* \Delta_{\widetilde{F}^{(k)}} + \Delta_{\widetilde{F}^{(k)}}{}^{\mathrm{T}} \Lambda^* + \Delta_2^{(k)}\right]_{ij} = \left[X^{(k)\mathrm{T}} A_\Delta^{(k)} X^{(k)}\right]_{ij} & (\text{otherwise}) \end{cases} \tag{35}$$

$$A_\Delta^{(k)} := A(\boldsymbol{c}^*) - A(\boldsymbol{c}^{(k+1)}), \quad \|\Delta_1^{(k)}\| \leq \|F^{(k)}\|^2, \quad \|\Delta_2^{(k)}\| \leq \|\Lambda^*\| \|F^{(k)}\|^2$$

For the convergence analysis, define $\bar{J}^{(k)}$ as $[\bar{J}^{(k)}]_{ij} = \boldsymbol{y}_i^{(k)\mathrm{T}} A_j \boldsymbol{y}_i^{(k)}$ in a similar manner as line 4 in Algorithm 1. Suppose that $\bar{J}^{(k)}$ is nonsingular. Then, we have

$$\|\bar{J}^{(k)-1}\| \sqrt{\sum_{j=1}^{n} \|A_j\|^2} \geq 1$$

because

$$\|\bar{J}^{(k)-1}\|^{-1} \leq \sqrt{\sum_{j=1}^{n} |\boldsymbol{y}_i^{(k)^{\mathrm{T}}} A_j \boldsymbol{y}_i^{(k)}|^2} \leq \sqrt{\sum_{j=1}^{n} \|A_j\|^2}$$

for any $i = 1, \ldots, n$. Using $\bar{J}^{(k)}$, we introduce

$$\alpha^{(k)} := \sqrt{n}\|\bar{J}^{(k)-1}\|\sqrt{\sum_{\ell=1}^{n} \|A_\ell\|^2} \geq \sqrt{n}. \tag{36}$$

If all the prescribe eigenvalues are distinct, $\bar{J}^{(k)}$ and $\alpha^{(k)}$ are independent of k. As a result, a condition of the convergence is written as

$$\|E^{(k)}\| \leq \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{6n\|\Lambda^*\|(1+\alpha)}$$

in [1, Theorem 1], where $\alpha = \alpha^{(k)}$ ($k = 0, 1, \ldots$). In the following, we prove the convergence under a similar condition, where the right-hand side is changed to

$$\frac{1}{3} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{6n\|\Lambda^*\|(1+\alpha^{(k)})},$$

depending on a constant 3 in (28). First, we prove the next lemma analogously to [1, §4].

Lemma 3. *Let $A_0, \ldots, A_n$ be real symmetric $n \times n$ matrices and $\lambda_1^* \leq \cdots \leq \lambda_n^*$ be prescribed eigenvalues. Suppose that Algorithm 1 is applied to $X^{(0)} \in \mathbb{R}^{n \times n}$. Moreover, for some k, suppose that*

$$\|F^{(k)}\| \leq \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1+\alpha^{(k)})}, \tag{37}$$

where $F^{(k)}$ is defined as Lemma 1, and $\alpha^{(k)}$ is defined as (36). For the computed $X^{(k+1)}$, define $G^{(k+1)}$ such that

$$X^{(k+1)} = Y^{(k)}(I + G^{(k+1)}). \tag{38}$$

Then, we obtain

$$\|G^{(k+1)}\| \leq \left(\frac{2n\|\Lambda^*\|(1+\alpha^{(k)})(1+\|F^{(k)}\|)}{\beta^{(k)} \min_{i \neq j} |\lambda_i^* - \lambda_j^*|} + 1\right)\|F^{(k)}\|^2, \tag{39}$$

$$\|F^{(k+1)}\| \leq 3\|G^{(k+1)}\|, \tag{40}$$

where

$$\beta^{(k)} := 1 - \alpha^{(k)}(2 + \|F^{(k)}\|)\|F^{(k)}\| \geq \rho_1 := \frac{575}{648}. \tag{41}$$

Proof. Noting (38) and

$$X^{(k+1)} = X^{(k)}(I - \widetilde{F}^{(k)}) = Y^{(k)}(I + F^{(k)})(I - \widetilde{F}^{(k)}),$$

we see

$$G^{(k+1)} = F^{(k)} - \widetilde{F}^{(k)} + F^{(k)}(F^{(k)} - \widetilde{F}^{(k)}) + F^{(k)2}. \quad (42)$$

It then follows that

$$\|G^{(k+1)}\| \leq (1 + \|F^{(k)}\|)\|\widetilde{F}^{(k)} - F^{(k)}\| + \|F^{(k)}\|^2. \quad (43)$$

Hence, to prove (39), we estimate $\|\widetilde{F}^{(k)} - F^{(k)}\|$.

First, we estimate the diagonal elements of $\widetilde{F}^{(k)} - F^{(k)}$. We see

$$|[\Delta_{\widetilde{F}^{(k)}}]_{ii}| = |[\widetilde{F}^{(k)}]_{ii} - [F^{(k)}]_{ii}| = \frac{|[\Delta_1^{(k)}]_{ii}|}{2} \leq \frac{\|F^{(k)}\|^2}{2} \quad (i = 1, \ldots, n) \quad (44)$$

from the diagonal elements in (34). In addition, for the off-diagonal elements corresponding to multiple eigenvalues $\lambda_i^* = \lambda_j^*$, we have

$$|[\Delta_{\widetilde{F}^{(k)}}]_{ij}| = |[\widetilde{F}^{(k)}]_{ij} - [F^{(k)}]_{ij}| = \frac{|[\Delta_1^{(k)}]_{ij}|}{2} \leq \frac{\|F^{(k)}\|^2}{2} \quad (i \neq j,\ \lambda_i^* = \lambda_j^*) \quad (45)$$

from (34) and the first equation in (35).

Next, we discuss $\boldsymbol{c}^{(k+1)}$ using the second equation in (35). In the left-hand side, we have

$$|[\Lambda^*(F^{(k)} - \widetilde{F}^{(k)}) + (F^{(k)\mathrm{T}} - \widetilde{F}^{(k)\mathrm{T}})\Lambda^* + \Delta_2^{(k)}]_{ii}| \leq \|\Lambda^*\|\|\Delta_1^{(k)}\| + \|\Delta_2^{(k)}\|$$

from (44). It then follows that

$$\begin{aligned}&\sqrt{\sum_{i=1}^{n} |[\Lambda^*(F^{(k)} - \widetilde{F}^{(k)}) + (F^{(k)\mathrm{T}} - \widetilde{F}^{(k)\mathrm{T}})\Lambda^* + \Delta_2^{(k)}]_{ii}|^2} \\ &\leq \sqrt{n}(\|\Lambda^*\|\|\Delta_1^{(k)}\| + \|\Delta_2^{(k)}\|).\end{aligned}$$

Therefore, using $J^{(k)}$ as in (22) and the diagonal elements of the second equation in (35), we obtain

$$\begin{aligned}\|\boldsymbol{c}^{(k+1)} - \boldsymbol{c}^*\| &\leq \|J^{(k)-1}\|\sqrt{n}(\|\Lambda^*\|\|\Delta_1^{(k)}\| + \|\Delta_2^{(k)}\|) \\ &\leq 2\|J^{(k)-1}\|\sqrt{n}\|\Lambda^*\|\|F^{(k)}\|^2. \quad (46)\end{aligned}$$

Concerning $\|J^{(k)-1}\|$, noting $\boldsymbol{x}_i^{(k)} = \boldsymbol{y}_i^{(k)} + \sum_{\ell=1}^{n}[F^{(k)}]_{\ell i}\boldsymbol{y}_\ell^{(k)}$ from the definition in (10), we see

$$\begin{aligned}|[\bar{J}^{(k)}]_{ij} - [J^{(k)}]_{ij}| &= |\boldsymbol{y}_i^{(k)\mathrm{T}} A_j \boldsymbol{y}_i^{(k)} - \boldsymbol{x}_i^{(k)\mathrm{T}} A_j \boldsymbol{x}_i^{(k)}| \\ &= |2\boldsymbol{y}_i^{(k)\mathrm{T}} A_j \sum_{\ell=1}^{n}[F^{(k)}]_{\ell i}\boldsymbol{y}_\ell^{(k)} + \sum_{\ell=1}^{n}[F^{(k)}]_{\ell i}\boldsymbol{y}_\ell^{(k)\mathrm{T}} A_j \sum_{\ell=1}^{n}[F^{(k)}]_{\ell i}\boldsymbol{y}_\ell^{(k)}| \\ &\leq (2 + \|F^{(k)}\|)\|F^{(k)}\|\|A_j\|\end{aligned}$$

from $\| \sum_{\ell=1}^{n} [F^{(k)}]_{\ell i} \boldsymbol{y}_\ell^{(k)} \| \leq \|F^{(k)}\|$. Using the Weyl's inequality for singular values, we have

$$\begin{aligned}
\|{J^{(k)}}^{-1}\|^{-1} &\geq \|\bar{J}^{(k)-1}\|^{-1} - \sqrt{\sum_{1\leq i,j \leq n} |[\bar{J}^{(k)}]_{ij} - [J^{(k)}]_{ij}|^2} \\
&\geq \|\bar{J}^{(k)-1}\|^{-1} - \sqrt{n}(2 + \|F^{(k)}\|)\|F^{(k)}\| \sqrt{\sum_{\ell=1}^{n} \|A_\ell\|^2} \\
&= \|\bar{J}^{(k)-1}\|^{-1} \left(1 - \alpha^{(k)}(2 + \|F^{(k)}\|)\|F^{(k)}\|\right).
\end{aligned}$$

We prove here that $1 - \alpha^{(k)}(2 + \|F^{(k)}\|)\|F^{(k)}\|$ in the right-hand side is positive. Since we assume (37), we have

$$\|F^{(k)}\| \leq \frac{1}{n} \cdot \frac{1}{9(1 + \alpha^{(k)})} \leq \min(1/36, 1/18\alpha^{(k)}) \tag{47}$$

for $n \geq 2$ and $\alpha^{(k)} \geq 1$. Hence, we see

$$1 - \alpha^{(k)}(2 + \|F^{(k)}\|)\|F^{(k)}\| \geq 1 - (2 + 1/36)/18 = \frac{575}{648}.$$

Thus, we obtain (41) and

$$\|{J^{(k)}}^{-1}\| \leq \|\bar{J}^{(k)-1}\| \left(1 - \alpha^{(k)}(2 + \|F^{(k)}\|)\|F^{(k)}\|\right)^{-1} = \frac{\|\bar{J}^{(k)-1}\|}{\beta^{(k)}}. \tag{48}$$

Using the inequalities (46) and (48), we estimate the off-diagonal elements of $\widetilde{F}^{(k)} - F^{(k)}$ corresponding to $\lambda_i^* \neq \lambda_j^*$ $(1 \leq i, j \leq n)$. Similarly to (25), we have

$$\begin{aligned}
&|[\widetilde{F}^{(k)}]_{ij} - [F^{(k)}]_{ij}| \\
&\leq \frac{|\lambda_j^*||[\Delta_1^{(k)}]_{ij}| + |[\Delta_2^{(k)}]_{ij}| + |\sum_{\ell=1}^{n}(c_\ell^{(k+1)} - c_\ell^*)\boldsymbol{x}_i^{(k)\mathrm{T}} A_\ell \boldsymbol{x}_j^{(k)}|}{|\lambda_i^* - \lambda_j^*|}
\end{aligned} \tag{49}$$

from (34) and the second equation in (35). In addition,

$$\begin{aligned}
&|\sum_{\ell=1}^{n}(c_\ell^{(k+1)} - c_\ell^*)\boldsymbol{x}_i^{(k)\mathrm{T}} A_\ell \boldsymbol{x}_j^{(k)}| \\
&\leq \sum_{\ell=1}^{n} |c_\ell^{(k+1)} - c_\ell^*| \|A_\ell\| (1 + \|F^{(k)}\|)^2 \\
&\leq (1 + \|F^{(k)}\|)^2 \|\boldsymbol{c}^{(k+1)} - \boldsymbol{c}^*\| \sqrt{\sum_{\ell=1}^{n} \|A_\ell\|^2}.
\end{aligned} \tag{50}$$

Therefore, we have

$$
\begin{aligned}
&|[\widetilde{F}^{(k)}]_{ij} - [F^{(k)}]_{ij}| \\
&\le \frac{2\|\Lambda^*\|\|F^{(k)}\|^2 + (1+\|F^{(k)}\|)^2\|\boldsymbol{c}^{(k+1)} - \boldsymbol{c}^*\|\sqrt{\sum_{\ell=1}^n \|A_\ell\|^2}}{|\lambda_i^* - \lambda_j^*|} \\
&\le \frac{2\|\Lambda^*\|\|F^{(k)}\|^2(1+\sqrt{n}\|{J^{(k)}}^{-1}\|(1+\|F^{(k)}\|)^2\sqrt{\sum_{\ell=1}^n \|A_\ell\|^2})}{|\lambda_i^* - \lambda_j^*|} \\
&\le \frac{2\|\Lambda^*\|}{\min_{i\neq j}|\lambda_i^* - \lambda_j^*|}\left(1 + \frac{\alpha^{(k)}(1+\|F^{(k)}\|)^2}{1-\alpha^{(k)}(2+\|F^{(k)}\|)\|F^{(k)}\|}\right)\|F^{(k)}\|^2 \\
&\le \frac{2\|\Lambda^*\|(1+\alpha^{(k)})}{\beta^{(k)}\min_{i\neq j}|\lambda_i^* - \lambda_j^*|}\|F^{(k)}\|^2,
\end{aligned}
$$

where the first inequality is due to (49) and (50), the second inequality is due to (46), the third inequality is due to (36) and (48), and the last inequality is due to the definition of $\beta^{(k)}$ in (41). Using (44), (45), and $\|\widetilde{F}^{(k)} - F^{(k)}\| \le \sqrt{\sum_{i,j}|[\widetilde{F}^{(k)}]_{ij} - [F^{(k)}]_{ij}|^2}$, we have

$$
\|\widetilde{F}^{(k)} - F^{(k)}\| \le \frac{2n\|\Lambda^*\|(1+\alpha^{(k)})}{\beta^{(k)}\min_{\lambda_i^*\neq\lambda_j^*}|\lambda_i^* - \lambda_j^*|}\|F^{(k)}\|^2.
$$

In view of (43), we obtain (39). We see (40) from Lemma 2. □

From (39) and (40) in the above lemma, it is easy to see that

$$
\|F^{(k+1)}\| \le 3\left(\frac{2n\|\Lambda^*\|(1+\alpha^{(k)})(1+\|F^{(k)}\|)}{\beta^{(k)}\min_{\lambda_i^*\neq\lambda_j^*}|\lambda_i^* - \lambda_j^*|} + 1\right)\|F^{(k)}\|^2.
$$

If $\alpha^{(k)}$ for $k = 0, 1, \dots$ are fixed as in the situation where all the eigenvalues are distinct, the asymptotic quadratic convergence as $\|F^{(k)}\| \to 0$ is obvious. Otherwise, we require a rigorous analysis of $\{\alpha^{(k)}\}_{k=0}^\infty$. For this purpose, we show a key lemma to estimate an upper bound of $\{\alpha^{(k)}\}_{k=0}^\infty$.

Lemma 4. *Under the same assumptions as in Lemma 3, we have*

$$
\alpha^{(k+1)} \le \frac{\alpha^{(k)}}{1-\alpha^{(k)}(2+4\|G^{(k+1)}\|)\cdot 4\|G^{(k+1)}\|}. \tag{51}
$$

In addition,

$$
\rho_2 := \frac{3239}{20700}, \quad \|G^{(k+1)}\| \le \rho_2\|F^{(k)}\|. \tag{52}
$$

Proof. Let

$$Y^{(k+1)} = Y^{(k)}(I + \widetilde{G}^{(k+1)}).$$

Combined this with the estimation in (48) for $X^{(k)} = Y^{(k)}(I + F^{(k)})$, we have

$$\|\bar{J}^{(k+1)-1}\| \leq \|\bar{J}^{(k)-1}\| \left(1 - \alpha^{(k)}(2 + \|\widetilde{G}^{(k+1)}\|)\|\widetilde{G}^{(k+1)}\|\right)^{-1}. \tag{53}$$

To estimate $\|\widetilde{G}^{(k+1)}\|$, we use the relations in Lemma 3:

$$X^{(k+1)} = Y^{(k)}(I + G^{(k+1)}) = Y^{(k+1)}(I + F^{(k+1)}),$$

which implies

$$\|\widetilde{G}^{(k+1)}\| = \|Y^{(k+1)} - Y^{(k)}\| \leq \|F^{(k+1)}\| + \|G^{(k+1)}\| \leq 4\|G^{(k+1)}\|. \tag{54}$$

Therefore, noting (53) and the definition of $\alpha^{(k)}$ in (36), we obtain (51). Moreover, we see (52) from

$$\begin{aligned} \|G^{(k+1)}\| &\leq \left(\frac{2n\|\Lambda^*\|(1+\alpha^{(k)})\|F^{(k)}\|}{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|} \cdot \frac{(1 + \|F^{(k)}\|)}{\beta^{(k)}} + \|F^{(k)}\|\right) \|F^{(k)}\| \\ &\leq \left(\frac{1}{9} \cdot \frac{648}{575} \cdot (1 + \frac{1}{36}) + \frac{1}{36}\right) \|F^{(k)}\|, \end{aligned}$$

where the first inequality is due to (39), and the second inequality is due to (37), (41), and (47), respectively. □

Using the above lemmas, we have the next lemma that states a crucial relationship between $F^{(k)}$ and $\alpha^{(k)}$.

Lemma 5. *Let $A_0, \ldots, A_n$ be real symmetric $n \times n$ matrices and $\lambda_1^* \leq \cdots \leq \lambda_n^*$ be prescribed eigenvalues. Suppose that Algorithm 1 is applied to $X^{(0)} \in \mathbb{R}^{n \times n}$. Moreover, suppose that there exist k and $\gamma^{(k)}$ such that*

$$0 \leq \gamma^{(k)} \leq 1, \quad \|F^{(k)}\| = \gamma^{(k)} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1 + \alpha^{(k)})}. \tag{55}$$

Then, we obtain

$$\rho_3 := \frac{3\rho_2}{\rho_1}, \quad \|F^{(k+1)}\| < \rho_3 \cdot \gamma^{(k)} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1 + \alpha^{(k+1)})}, \tag{56}$$

where $\rho_3 = 0.529 \cdots < 1$.

Proof. Similarly to (47), we have

$$\|F^{(k)}\| \leq \gamma^{(k)} \cdot \frac{1}{n} \cdot \frac{1}{9(1+\alpha^{(k)})} \leq \gamma^{(k)} \cdot \min(1/36, 1/18\alpha^{(k)}). \tag{57}$$

From Lemma 4, we have

$$\alpha^{(k+1)} \leq \frac{\alpha^{(k)}}{\beta^{(k)}} \leq \frac{\alpha^{(k)}}{\rho_1},$$

where $\beta^{(k)}$ and ρ_1 are defined in (41). It then follows that

$$\frac{1}{\alpha^{(k)}+1} < \frac{1}{\rho_1} \cdot \frac{1}{\alpha^{(k+1)}+1},$$

which implies

$$\gamma^{(k)} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1+\alpha^{(k)})} < \frac{\gamma^{(k)}}{\rho_1} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1+\alpha^{(k+1)})}.$$

Therefore, noting (40), (52), and (55), we have

$$\|F^{(k+1)}\| \leq 3\rho_2\|F^{(k)}\| < \frac{3\rho_2}{\rho_1} \cdot \gamma^{(k)} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1+\alpha^{(k+1)})},$$

which shows (56). □

Using the above lemmas, we prove the quadratic convergence of the proposed algorithm as follows.

Theorem 1. *Let $A_0, \ldots, A_n$ be real symmetric $n \times n$ matrices and $\lambda_1^* \leq \cdots \leq \lambda_n^*$ be prescribed eigenvalues. Suppose that Algorithm 1 is applied to $X^{(0)} \in \mathbb{R}^{n\times n}$. In addition, $F^{(k)}$ $(k = 0, 1, \ldots)$ are defined as in Lemma 1. Moreover, for some k, suppose that $F^{(k)}$ satisfies* (37)*. Then, we obtain*

$$\|F^{(k+\ell)}\| \leq (3\rho_2)^{\ell}\|F^{(k)}\| \quad (\ell = 0, 1, \ldots) \tag{58}$$

$$\limsup_{\ell\to\infty} \frac{\|F^{(k+\ell+1)}\|}{\|F^{(k+\ell)}\|^2} \leq 3\left(\frac{2n\|\Lambda^*\|(1+\rho_4\alpha^{(k)})}{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|} + 1\right), \tag{59}$$

where ρ_2 is defined as in (52) *and*

$$\rho_4 := \exp\left(\frac{73}{575} \cdot \frac{1}{1-\rho_3}\right) (= 1.309\cdots)$$

for ρ_3 defined as in (56)*.*

Proof. Define $\gamma^{(k+\ell)}$ $(\ell = 1, 2, \ldots)$ such that

$$\|F^{(k+\ell)}\| = \gamma^{(k+\ell)} \cdot \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1 + \alpha^{(k+\ell)})}$$

in the same manner as (55). Then, we see

$$\gamma^{(\ell+k)} \leq {\rho_3}^{\ell} \gamma^{(k)} \leq {\rho_3}^{\ell} \leq 1 \quad (\ell = 0, 1, \ldots) \tag{60}$$

from Lemma 5. Therefore, noting

$$\|F^{(k+\ell)}\| \leq \frac{\min_{\lambda_i^* \neq \lambda_j^*} |\lambda_i^* - \lambda_j^*|}{18n\|\Lambda^*\|(1 + \alpha^{(k+\ell)})} \quad (\ell = 0, 1, \ldots)$$

and Lemmas 3 and 4, we obtain (58). In addition, we see

$$\|F^{(k+\ell)}\| \leq \frac{{\rho_3}^{\ell}}{36}, \quad \alpha^{(k+\ell)}\|F^{(k+\ell)}\| \leq \frac{{\rho_3}^{\ell}}{18} \quad (\ell = 0, 1, \ldots) \tag{61}$$

from (57) and (60). Hence, we have

$$\begin{aligned}
\alpha^{(k+\ell+1)} &\leq \frac{\alpha^{(k+\ell)}}{1 - \alpha^{(k+\ell)}(2 + 4\|G^{(k+\ell+1)}\|) \cdot 4\|G^{(k+\ell+1)}\|} \\
&\leq \frac{\alpha^{(k+\ell)}}{1 - \alpha^{(k+\ell)}(2 + \|F^{(k+\ell)}\|)\|F^{(k+\ell)}\|} \\
&= \alpha^{(k+\ell)} \left(1 + \frac{\alpha^{(k+\ell)}(2 + \|F^{(k+\ell)}\|)\|F^{(k+\ell)}\|}{1 - \alpha^{(k+\ell)}(2 + \|F^{(k+\ell)}\|)\|F^{(k+\ell)}\|} \right) \\
&\leq \alpha^{(k+\ell)} \left(1 + \frac{648}{575} \cdot (2 + \frac{1}{36}) \cdot \frac{1}{18}{\rho_3}^{\ell} \right) \\
&\leq \alpha^{(k+\ell)} \exp\left(\frac{73}{575}{\rho_3}^{\ell} \right) \\
&\leq \alpha^{(k)} \exp\left(\frac{73}{575} \cdot \frac{1 - {\rho_3}^{\ell+1}}{1 - \rho_3} \right),
\end{aligned}$$

where the first inequality is due to (51), the second inequality is due to $4\|G^{(k+\ell+1)}\| \leq \|F^{(k+\ell)}\|$ from (52), and the third inequality is due to (41) and (61), respectively. It then follows that

$$\alpha^{(k+\ell)} \leq \alpha^{(k)} \exp\left(\frac{73}{575} \cdot \frac{1}{1 - \rho_3} \right), \quad \exp\left(\frac{73}{575} \cdot \frac{1}{1 - \rho_3} \right) = 1.309\cdots$$

for all $\ell = 0, 1, \ldots$. Therefore, using (39) and (40), we obtain (59). □

Here, we prove that there exist $\lim_{\ell \to \infty} Y^{(k+\ell)}$ and $\lim_{\ell \to \infty} X^{(k+\ell)}$. From (54), we see $\|Y^{(k+\ell)} - Y^{(k+\ell+1)}\|$ is quadratically convergent as $\ell \to \infty$. In other words, $\{\|Y^{(k+\ell)}\|\}_{\ell=0}^{\infty}$ is the Cauchy sequence, and hence there exists $Y^{(\infty)}$. In addition, there exists $X^{(\infty)}$ from $X^{(k)} = Y^{(k)}(I + F^{(k)})$ and $\|F^{(\infty)}\| = 0$.

Finally, noting the above convergence analysis, we show a simple extension of our result to inverse Hermitian eigenvalue problems. Let $A_0, A_1, \ldots, A_n \in \mathbb{C}^{n\times n}$ be Hermitian matrices. The purpose is to find a real vector $\boldsymbol{c}^* \in \mathbb{R}^n$ such that $A(\boldsymbol{c}^*)$ has prescribed real eigenvalues. If we replace the transpose with the conjugate transpose in Algorithm 1, this generalized version can be applied to the above inverse Hermitian eigenvalue problems. However, we must note that, for any diagonal unitary matrix U, X^*U is also an eigenvector matrix; there is a continuum of X^* even if all the eigenvalues are distinct. Since this property is completely different from the real case, below we analyze the details. For simplicity, let us consider the situation where the prescribed eigenvalues are all distinct. As shown above, since X^* is not unique, $E^{(k)}$ is not unique for a fixed $X^{(k)}$ for any k. The lack of the uniqueness is relevant the diagonal elements for $\widetilde{E}^{(k)}$ given by

$$\widetilde{E}^{(k)\mathrm{H}} + \widetilde{E}^{(k)} = X^{(k)\mathrm{H}}X^{(k)} - I$$

corresponding to (5), where the symbol H denotes the conjugate transpose. It is easy to see that the diagonal elements for $\widetilde{E}^{(k)}$ are not uniquely determined in $\mathbb{C}$. However, Algorithm 1 computes

$$[\widetilde{F}^{(k)}]_{ii} = \frac{[X^{(k)\mathrm{H}}X^{(k)} - I]_{ii}}{2} \in \mathbb{R} \tag{62}$$

for $i = 1, \ldots, n$ in line 3. Recall that we introduce $Y^{(k)} \in \{X^*\}$ in Section 2. Analogously, for any $\boldsymbol{x}_i^{(k)}$ for $i = 1, \ldots, n$, we consider an optimization problem:

$$\min \|\boldsymbol{x}_i^* - \boldsymbol{x}_i^{(k)}\| \text{ such that } \boldsymbol{x}_i^* \in \mathbb{C}^n \text{ with } \|\boldsymbol{x}_i^*\| = 1$$

for every $i = 1, \ldots, n$. Similarly to the optimization problem in (12), the solution vectors $\boldsymbol{y}_i^{(k)}$ $(i = 1, \ldots, n)$ of the above problems satisfy $\boldsymbol{y}_i^{(k)\mathrm{H}}\boldsymbol{x}_i^{(k)} \in \mathbb{R}$ for all $i = 1, \ldots, n$. Hence, for the eigenvector matrix $Y^{(k)} = [\boldsymbol{y}_1^{(k)}, \ldots, \boldsymbol{y}_n^{(k)}]$, we introduce $F^{(k)}$ as in Lemma 1. Note that the diagonal elements of $F^{(k)}$ are real from $\boldsymbol{y}_i^{(k)\mathrm{H}}\boldsymbol{x}_i^{(k)} \in \mathbb{R}$ for all $i = 1, \ldots, n$. Thus, we see that the generalized version of Algorithm 1 computes $\widetilde{F}^{(k)}$ approximating $F^{(k)}$ as in (62). Therefore, the convergence results in Section 3 can be extended to the above Hermitian case. Moreover, the above discussion can be easily generalized to an arbitrary set of prescribed eigenvalues $\lambda_1^* \le \cdots \le \lambda_n^*$.

4 Comparison with previous work

In this section, to clarify the strength of our convergence analysis, we first review some previous work.

More precisely, we discuss convergence analysis for various quadratically convergent methods originally presented in [14, §2]; see [2, 3, 4, 5, 6, 7, 8] for the details of their algorithm developments and the corresponding convergence theory. All of the existing quadratically convergent methods require to solve linear systems. The coefficient matrices $J(X^{(k)}) \in \mathbb{R}^{n\times n}$ $(k = 0, 1, \ldots)$ are defined as

$$[J(X^{(k)})]_{ij} := \boldsymbol{x}_i^{(k)\mathrm{T}} A_j \boldsymbol{x}_i^{(k)} \quad (k = 0, 1, \ldots),$$

where $X^{(k)} := [\boldsymbol{x}_1^{(k)}, \cdots, \boldsymbol{x}_n^{(k)}]$ for $k = 0, 1, \ldots$ are approximated eigenvector matrices in the iterative methods. Hence, one may think

$$[J(X^*)]_{ij} := \boldsymbol{x}_i^{*\mathrm{T}} A_j \boldsymbol{x}_i^*, \quad \sup_{X^*} \|J(X^*)^{-1}\|$$

for the convergence analysis. However, in general, the above supremum does not exist as shown in [14, §3.1]. Since the convergence proof is not easy due to the above singularity of $J(X^*)$ for some X^*, the following inequalities

$$\|J(X^{(k)})^{-1}\| < \infty \ (k = 0, 1, \ldots), \quad \limsup_{k\to\infty} \|J(X^{(k)})^{-1}\| < \infty \tag{63}$$

are always assumed for the proof of the quadratic convergence also in recent papers [17, 18, 19]. One may think that the above conditions as in (63) are not so restrictive because the set of the singular matrices are almost surely avoided in the iterative process. In fact, the quadratic convergence is usually observed in numerical tests even if multiple eigenvalues are present. Hence, from the mathematical point of view, many efforts have been made to remove the assumptions in (63) that must be satisfied automatically. For example, noting that $X^{*\mathrm{T}} A(\boldsymbol{c}^*) X^* = \Lambda^*$ can be considered an overdetermined system of equations, Friedland, Nocedal, and Overton proposed the modified versions in [14, §3.2] applied to multiple eigenvalues. The idea is to reduce the number of the specified eigenvalues depending on the number of multiple eigenvalues. The quadratic convergence is proved under more natural assumptions in [14, §3.3] as in the problem where the specified eigenvalues are all simple, i.e., $\lambda_1^* < \cdots < \lambda_n^*$. However, one difficulty remains as shown in [14, §3.2]. If some eigenvalues that are not specified are actually multiple, a tolerance parameter is required for avoiding the divergence of $\|X^{(k)}\|$ $(k = 0, 1, \ldots)$. In addition, recall that the assumptions in (63) cannot be removed for the proof of the quadratic convergence of unmodified methods.

With such a background, we provide a different formulation for the proof of quadratic convergence in the previous section. Intuitively, if $X^{(k)}$ for some k is close to some X^* associated with $J(X^*)$ whose condition number is not so large, then $\{X^{(k+\ell)}\}_{\ell=0}^{\infty}$ should converge to some neighborhood of X^*. From such a perspective, we first construct an ideal matrix $Y^{(k)} \in \{X^*\}$

depending on $X^{(k)}$ as in Lemma 1. Next, we suppose that $\|F^{(k)}\|$, defined as in Lemma 1, is sufficiently small compared with $\|J(Y^{(k)})^{-1}\|$ as in (37). In other words, our convergence proof only requires the assumption on some k as in (37), resulting in Theorem 1 that ensures quadratic convergence. This formulation is the crucial strength of our convergence analysis. Note that, if we assume (63), the quadratic convergence is immediately proved from (39) and (40) in Lemma 3 without Lemmas 4 and 5 that state important properties of $\|F^{(k)}\|$ and $\|J(Y^{(k)})^{-1}\|$ for $k = 0, 1, \ldots$.

From the above mathematical discussion, one may notice that a concept of relative generalized Jacobian matrices is introduced in [20]. On the basis of the relative generalized Jacobian matrices, the quadratic convergence for some existing algorithms is proved as follows. Let

$$\mathcal{D} = \{\boldsymbol{c} \in \mathbb{R}^n \mid \text{Eigenvalues of } A(\boldsymbol{c}) \text{ are all distinct}\}.$$

In addition, let $X^*(\boldsymbol{c}) = [\boldsymbol{x}_1^*(\boldsymbol{c}), \ldots, \boldsymbol{x}_n^*(\boldsymbol{c})]$ denote an eigenvector matrix of $A(\boldsymbol{c})$ for $\boldsymbol{c} \in \mathcal{D}$. Moreover, let $[J^*(\boldsymbol{c})]_{ij} := \boldsymbol{x}_i^*(\boldsymbol{c})^{\mathrm{T}} A_j \boldsymbol{x}_i^*(\boldsymbol{c})$ for all $1 \le i, j \le n$. Then, the relative generalized Jacobian matrices in [20] are defined as

$$\{J^* := \lim_{k\to\infty} J^*(\boldsymbol{c}^{(k)}) \text{ with } \{\boldsymbol{c}^{(k)}\}_{k=0,1,\ldots} \subset \mathcal{D} \text{ and } \boldsymbol{c}^{(\infty)} = \boldsymbol{c}^*\}. \tag{64}$$

According to [17, 19, 20], quadratic convergence for some methods is proved if all of $\{J^*\}$ are nonsingular, where such assumptions appear to be almost surely satisfied.

The question then arises: in general, all of $\{J^*\}$ are nonsingular indeed? The answer with mathematical rigor is not explicitly written in [20]. Alternatively, the following example is shown. To see the example, let

$$A_0 = O,\ A_1 = I,\ A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \lambda_1^* = \lambda_2^* = 1,$$

where the solution is $\boldsymbol{c}^* = [1,\ 0]^{\mathrm{T}}$. Obviously, $\mathcal{D} = \{\boldsymbol{c} \in \mathbb{R}^2 \mid c_2 \neq 0\}$. Thus, the relative Jacobian matrices $\{J^*\}$ are

$$\left\{ \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \right\},$$

which are nonsingular.

To more deeply investigate the features of the relative Jacobian matrices, let us consider the following inverse eigenvalue problem:

$$A_0 = O,\ A_1 = \begin{bmatrix} 1 & 0 \\ 0 & t \end{bmatrix},\ A_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \lambda_1^* = \lambda_2^* = 0,$$

where the solution is $\boldsymbol{c}^* = [0,\ 0]^{\mathrm{T}}$. If $t = 1$, the relative Jacobians are the same as the previous example. Otherwise, $\mathcal{D} = \{\boldsymbol{c} \in \mathbb{R}^2 \mid \boldsymbol{c} \neq \boldsymbol{c}^*\}$. Thus, for $\boldsymbol{c} = [c_1,\ 0]^{\mathrm{T}}$ ($c_1 \neq 0$), $\{J^*(\boldsymbol{c})\}$ are

$$\left\{ \begin{bmatrix} 1 & 0 \\ t & 0 \end{bmatrix}, \begin{bmatrix} t & 0 \\ 1 & 0 \end{bmatrix} \right\}, \tag{65}$$

which implies that some relative generalized Jacobian matrices are singular. Here, to consider any eigenvector matrix, let

$$\boldsymbol{q}_1 = \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix},\ \boldsymbol{q}_2 = \begin{bmatrix} -\sin(\theta) \\ \cos(\theta) \end{bmatrix},\ Q = [\boldsymbol{q}_1,\ \boldsymbol{q}_2].$$

Noting

$$J^*(Q) := \begin{bmatrix} \boldsymbol{q}_1^{\mathrm{T}} A_1 \boldsymbol{q}_1 & \boldsymbol{q}_1^{\mathrm{T}} A_2 \boldsymbol{q}_1 \\ \boldsymbol{q}_2^{\mathrm{T}} A_1 \boldsymbol{q}_2 & \boldsymbol{q}_2^{\mathrm{T}} A_2 \boldsymbol{q}_2 \end{bmatrix} = \begin{bmatrix} \cos^2(\theta) + t\sin^2(\theta) & 2\cos(\theta)\sin(\theta) \\ t\cos^2(\theta) + \sin^2(\theta) & -2\cos(\theta)\sin(\theta) \end{bmatrix},$$

we see

$$\det(J^*(Q)) = -2(1+t)\cos(\theta)\sin(\theta).$$

If $t = -1$, then $J^*(Q)$ is always singular. Otherwise, in general, $J^*(Q)$ is nonsingular, unless $\cos(\theta)\sin(\theta) = 0$ associated with $\boldsymbol{c} = [c_1,\ 0]^{\mathrm{T}}$ ($c_1 \neq 0$). In other words, if we chose a vector $\boldsymbol{c} = [c_1,\ c_2]^{\mathrm{T}}$ ($c_2 \neq 0$), $J^*(Q)$ is nonsingular, and hence the convergence from such a direction $\boldsymbol{c}$ is expected, even though some relative Jacobian matrices are singular as in (65). This indicates that the above assumption for the relative Jacobian matrices $\{J^*\}$ in (64) might be too strong to ensure (63) for some fixed $\{X^{(k)}\}_{k=0}^{\infty}$. It is not required that all of $\{J^*\}$ in (64) concerning *any* sequence of $\{\boldsymbol{c}^{(k)}\}_{k=0,1,\ldots}$ are assumed to be nonsingular.

After all, from the mathematical point of view, the actual convergence behavior should be verified using a distance between an approximate solution $X^{(k)}$ and some exact solution, such as $Y^{(k)} \in \{X^*\}$ in the previous section. In this sense, our convergence analysis is straightforward and convincing. Theorem 1 ensures the quadratic convergence under the assumption on some k as in (37) concerning $X^{(k)},\ Y^{(k)} \in \{X^*\}$, and $\bar{J}^{(k)}$. Again we stress that this formulation is the crucial strength of our convergence analysis.

5 Numerical test

In this section, we report a numerical result to illustrate the convergence theory for the proposed algorithm. The following test was performed in MATLAB. We used a typical problem in [14, Example 2], where the target

Table 1: Convergence of $\|F^{(k)}\|$ and $\|\boldsymbol{c}^{(k)} - \boldsymbol{c}^*\|$

k	$\|F^{(k)}\|$	$\|\boldsymbol{c}^{(k)} - \boldsymbol{c}^*\|$
0	9.41E−02	1.22E−02
1	1.66E−02	1.77E−02
2	4.29E−04	3.69E−04
3	6.45E−07	6.63E−07
4	1.15E−12	1.03E−12

matrix $A(\boldsymbol{c}^*)$ has multiple eigenvalues. First, let

$$V := \begin{bmatrix} 1 & -1 & -3 & -5 & -6 \\ 1 & 1 & -2 & -5 & -17 \\ 1 & -1 & -1 & 5 & 18 \\ 1 & 1 & 1 & 2 & 0 \\ 1 & -1 & 2 & 0 & 1 \\ 1 & 1 & 3 & 0 & -1 \\ 2.5 & 0.2 & 0.3 & 0.5 & 0.6 \\ 2 & -0.2 & 0.3 & 0.5 & 0.8 \end{bmatrix}.$$

Next, we generate $B = I + VV^{\mathrm{T}}$ that has 3 multiple eigenvalues $\lambda_1^* = \lambda_2^* = \lambda_3^* = 1$. The other eigenvalues are all simple. In addition, let $A_0 = O$, and define A_i for $i = 1, 2, \dots, 8$ as

$$A_i = [B]_{ii}\mathbf{e}_i\mathbf{e}_i^{\mathrm{T}} + \sum_{j=1}^{i-1}[B]_{ij}(\mathbf{e}_i\mathbf{e}_j^{\mathrm{T}} + \mathbf{e}_j\mathbf{e}_i^{\mathrm{T}}) \quad (i = 1, 2, \dots, 8),$$

where $\mathbf{e}_i$ are the ith columns of $I \in \mathbb{R}^{8\times 8}$ for $i = 1, 2, \dots, 8$. We suppose $\boldsymbol{c}^* = [1, 1, \dots, 1]^{\mathrm{T}}$ and use an initial guess $\boldsymbol{c}^{(0)} = \boldsymbol{c}^* + \boldsymbol{\xi}$, where each element of $\boldsymbol{\xi}$ is chosen by a random number uniformly distributed between -10^{-2} and 10^{-2}. Let the corresponding initial matrix $X^{(0)}$ be an eigenvector matrix of $A(\boldsymbol{c}^{(0)})$, which is computed by the MATLAB build-in function `eig`.

The numerical result is displayed in Table 1. The quadratic convergence can be observed in some neighborhood of the exact solutions.

6 Concluding remarks

In this paper, improving the latest algorithm in [1], we have derived the new algorithm adapted to an arbitrary set of prescribed eigenvalues, and then proved the quadratic convergence under a technical assumption. More specifically, we have shown a straightforward and sophisticated approach to multiple eigenvalues using the orthogonal Procrustes problem [15, §6.4.1]. Such an idea based on the polar decomposition is found in [16] that presents an efficient iterative refinement algorithm for symmetric eigenvalue problems. As shown in Section 4, it is worth noting that the quadratic convergence is theoretically guaranteed under a natural assumption on some iteration number k as in Theorem 1. It is a different formulation from the previous work for the other quadratically convergent methods in the research fields of inverse eigenvalue problems.

Acknowledgement
This study was supported by KAKENHI Grant Number 17K14143.

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