SIAM J. MATRIX ANAL. APPL.
Vol. 35, No. 3, pp. 1205–1225
© 2014 Society for Industrial and Applied Mathematics

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

FAST ENCLOSURE FOR ALL EIGENVALUES AND INVARIANT SUBSPACES IN GENERALIZED EIGENVALUE PROBLEMS*

SHINYA MIYAJIMA†

Abstract. Two fast algorithms for enclosing all eigenvalues and invariant subspaces in generalized eigenvalue problems are proposed. In these algorithms, individual eigenvectors and invariant subspaces are enclosed when eigenvalues are well separated and closely clustered, respectively. The first algorithm involves only cubic complexity and automatically determines eigenvalue clusters. The second algorithm is applicable even for defective eigenvalues. Numerical results show the properties of the proposed algorithms.

Key words. generalized eigenvalue problem, invariant subspace, numerical enclosure

AMS subject classifications. 65F05, 65G20, 65G50

DOI. 10.1137/140953150

1. Introduction.

In this paper, we are concerned with the accuracy of numerically computed solutions in the generalized eigenvalue problems

$$Ax = \lambda Bx, \qquad A, B \in \mathbb{C}^{n\times n}, \quad \lambda \in \mathbb{C}, \quad x \in \mathbb{C}^n, \tag{1.1}$$

where λ is an eigenvalue, $x \neq 0$ is an eigenvector corresponding to λ, and B is nonsingular. Let $k \leq n$, and $P_s \in \mathbb{C}^{n\times k}$ and $\Lambda \in \mathbb{C}^{k\times k}$ satisfy $AP_s = BP_s\Lambda$, where Λ is not necessarily diagonal. The eigenvalues of Λ are those of (1.1), and span(P_s) is called the invariant subspace in (1.1) corresponding to these eigenvalues. The eigenvectors in (1.1) corresponding to these eigenvalues are included in this subspace (see [1], e.g.).

We consider enclosing eigenvalues and invariant subspaces using floating point operations. There are several algorithms for enclosing them, e.g., [2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. The algorithms in [2, 3, 4, 7, 10, 11] are applicable when A is Hermitian and B is Hermitian positive definite, and require $\mathcal{O}(n^3)$ operations. The algorithms in [2], [3], [10], and [11] are based on Temple quotients, variational principles, and Cholesky and $\mathrm{LDL}^{\mathrm{T}}$ factorizations, respectively, and enclose *a few specified eigenvalues*. The algorithms in [4] and [7] are based on perturbation theories and enclose *all eigenvalues* and *all eigenvalues and invariant subspaces*, respectively. The algorithms in [5, 6, 8, 9] are applicable even when A is not Hermitian and/or B is not Hermitian positive definite and also require $\mathcal{O}(n^3)$ operations. The algorithms in [5, 6] are based on the perturbation theories and enclose *all eigenvalues*. The algorithms in [8] and [9] are based on nonlinear equations arising from (1.1) and $AP_s = BP_s\Lambda$, respectively, and enclose *a few specified eigenvalues and invariant subspaces*. The algorithm in [9] is applicable even for defective eigenvalues, although the other algorithms are not applicable in this case.

The purpose of this paper is to propose two algorithms for enclosing *all eigenvalues and invariant subspaces*, which are applicable even to the non-Hermitian cases.

*Received by the editors January 17, 2014; accepted for publication (in revised form) by A. Frommer June 25, 2014; published electronically September 11, 2014. This research was partially supported by a grant-in-aid for scientific research (23560066, 2011–2015) from the Ministry of Education, Science, Sports and Culture of Japan.
http://www.siam.org/journals/simax/35-3/95315.html
†Faculty of Engineering, Gifu University, 501-1193, Japan (miyajima@gifu-u.ac.jp).

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

In these algorithms, the nonsingularity of B is not assumed but proved, and individual eigenvectors and invariant subspaces are enclosed when eigenvalues are well separated and closely clustered, respectively. The first and second algorithms are based on nonlinear equations obtained by transforming $AP_s = BP_s\Lambda$ utilizing generalized eigendecomposition (GED) and block diagonalization (BD) analogous to [12], respectively. Let m_1 and m_2 be numbers of well-separated eigenvalues and eigenvalue clusters, respectively, and $m := m_1 + m_2$. All the eigenvalues and invariant subspaces can be enclosed by repeatedly executing the algorithms in [8, 9]. If we adopt this approach, on the other hand, $\mathcal{O}(mn^3)$ operations are required. However the proposed algorithms do not require $\mathcal{O}(mn^3)$ operations (see sections 3.4 and 4.3). This efficiency comes from exploitation of sparse matrices obtained by the GED or BD. The first algorithm involves only $\mathcal{O}(n^3)$ operations and first computes n disks containing all the eigenvalues based on the Gershgorin theorem. If k of the disks form a connected domain which is isolated from the other disks, therefore, this domain contains precisely k eigenvalues. By utilizing this property, this algorithm automatically determines eigenvalue clusters, whereas the algorithm in [9] requires users to determine them. The second algorithm is applicable even for defective eigenvalues. We finally report numerical results to observe the properties of the proposed two algorithms.

2. Preliminaries. In this section, we introduce notation and theories utilized hereafter. For $M \in \mathbb{C}^{m\times n}$, let M_{ij} and $M_{:j}$ denote the (i,j) element and the jth column of M, respectively, $|M| := (|M_{ij}|)$, $M^T := (M_{ji})$, $\|M\|_\infty := \max_i \sum_j |M_{ij}|$, $\|M\|_{\mathrm{M}} := \max_{i,j} |M_{ij}|$, and $\mathrm{vec}(M) := (M_{:1}^T, \ldots, M_{:n}^T)^T$. When $m = n$ in particular, $\rho(M)$ and $\overline{\rho}(M)$ denote the spectral radius of M and an upper bound of $\rho(M)$, respectively. For $M, N \in \mathbb{R}^{m\times n}$, $M \le N$ means that $M_{ij} \le N_{ij}$ follows for all i and j. For $v \in \mathbb{C}^n$, v_i denotes the ith component of v. For $v, w \in \mathbb{C}^n$ with $\|w\|_\infty < 1$, define $\|v\|_w := \max_i(|v_i|/(1-|w_i|))$. Let I_n, $e^{(i)}$ and $\mathbb{1}$ be the $n\times n$ identity matrix, the ith column of I_n, and the column vector with proper dimension all of whose elements are 1, respectively. For $M^c \in \mathbb{C}^{m\times n}$ and $M^r \in \mathbb{R}^{m\times n}$, where M^r has nonnegative components, $\langle M^c, M^r\rangle$ denotes the interval matrix whose center and radius are M^c and M^r, respectively. When $m = n = 1$, especially, $\langle M^c, M^r\rangle$ geometrically means a disk in the complex plane. Let $\circ$ and $./$ be the pointwise multiplication and division, respectively. The notation $\mathrm{fl}(\cdot)$ and $\mathrm{fl}_\triangle(\cdot)$ denote results of floating point computations, where all operations inside parentheses are executed by ordinary floating point arithmetic in rounding to nearest and rounding toward $+\infty$ modes, respectively. The notation $\overline{\mathrm{fl}}(\cdot)$ denotes a rigorous upper bound of inside parentheses obtained by rounding mode controlled floating point computations. Let `eps`, `realmin`, $\otimes$ and $\mathbb{F}$ be machine epsilon, the smallest positive normalized floating point number (especially $\mathtt{eps} = 2^{-52}$ and $\mathtt{realmin} = 2^{-1022}$ in IEEE 754 double precision), the Kronecker product (see [13], e.g.) and the set of all floating point real numbers, respectively. For a Fréchet differentiable matrix function $F(X)$ where $X \in \mathbb{C}^{m\times n}$, denote the Fréchet derivative of F at X applied to the matrix H by $F'_X(H)$. We introduce Lemmas 2.1, 2.2, 2.3, and 2.5 and Corollary 2.4.

LEMMA 2.1 (e.g., Golub and Van Loan [1]). *For $S \in \mathbb{C}^{n\times n}$ and $1 \le p \le \infty$, if $\|S\|_p < 1$, $I_n - S$ is nonsingular.*

LEMMA 2.2 (e.g., Horn and Johnson [13]). *For any complex matrices K, L, M, and N with compatible sizes, it holds that $(K\otimes L)(M\otimes N) = (KM \otimes LN)$ and $\mathrm{vec}(LMN) = (N^T \otimes L)\mathrm{vec}(M)$.*

LEMMA 2.3 (Minamihata [14]). *Let $S \in \mathbb{C}^{n\times n}$, $f \in \mathbb{C}^n$ and $t := |S|\mathbb{1}$. If $\|t\|_\infty < 1$, then $I_n - S$ is nonsingular and $|(I_n - S)^{-1}||f| \le |f| + \|f\|_t t$ holds.*

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Proof. Lemma 2.1 and $\|S\|_\infty = \|t\|_\infty < 1$ give the nonsingularity of $I_n - S$. The Neumann series gives

$$\begin{aligned}|(I_n - S)^{-1}||f| &\le |f| + |S|(I_n + |S| + |S|^2 + \cdots)|f| = |f| + |S|(I_n - |S|)^{-1}|f| \\ &= |f| + |S|(I_n - |S|)^{-1}\left(\frac{|f|_1(1-t_1)}{1-t_1}, \ldots, \frac{|f|_n(1-t_n)}{1-t_n}\right)^T \\ &\le |f| + \|f\|_t|S|(I_n - |S|)^{-1}(\mathbb{1} - t) \\ &= |f| + \|f\|_t|S|(I_n - |S|)^{-1}(I_n - |S|)\mathbb{1} = |f| + \|f\|_t t. \qquad \square\end{aligned}$$

COROLLARY 2.4. *Let S and t be as in Lemma 2.3 and $F \in \mathbb{C}^{n\times k}$. Assume $\|t\|_\infty < 1$ and define $w := (\|F_{:1}\|_t, \ldots, \|F_{:k}\|_t)^T$. Then $I_n - S$ is nonsingular and $|(I_n - S)^{-1}||F| \le |F| + tw^T$ follows.*

Proof. The identity $|F| = (|F_{:1}|, \ldots, |F_{:k}|)$ and the applications of Lemma 2.3 to $|(I_n - S)^{-1}||F_{:j}|$, $j = 1, \ldots, k$, show the result. $\square$

LEMMA 2.5. *Let $M \in \mathbb{C}^{n\times n}$, $v \in \mathbb{C}^n$, and $v_i \ne 0\ \forall\ i$. Then $(M./(v\mathbb{1}^T))\mathbb{1} = (M\mathbb{1})./v$ holds.*

Proof. The result follows from $(M./(v\mathbb{1}^T))\mathbb{1} = \left(\sum_{i=1}^n M_{1i}/v_1, \ldots, \sum_{i=1}^n M_{ni}/v_n\right)^T = (M\mathbb{1})./v$. $\square$

3. Enclosure utilizing GED. In this section, we establish theories for enclosing all the eigenvalues and invariant subspaces based on the GED $AX = BXD$, $X, D \in \mathbb{C}^{n\times n}$, where D is diagonal. If B is nonsingular (this can be verified by the algorithm in this section), the GED exists, although X is not always nonsingular. We also propose an algorithm for enclosing them based on the established theories. In section 3.1, we cite and construct a previous and a new theory for computing n disks containing all eigenvalues, respectively. In section 3.2, we present a theory for enclosing an individual eigenvector in the case when one of the disks is isolated from the other disks. In section 3.3, we establish a theory for enclosing invariant subspaces in the case when some of the disks are connected. The algorithm based on these theories is proposed in section 3.4. Let $\tilde{X}$ and $\tilde{D}$ be the numerical results for X and D, respectively, and let Y be an approximation of $(B\tilde{X})^{-1}$. Then we can expect $A\tilde{X} - B\tilde{X}\tilde{D} \approx 0$ and $I_n - YB\tilde{X} \approx 0$.

3.1. Disks containing all eigenvalues. We cite Theorem 3.1 as the previous theory for enclosing all the eigenvalues. Corollary 3.2 and Lemma 3.4 are presented for enclosing them and clarifying the advantage of Corollary 3.2, respectively.

THEOREM 3.1 (Miyajima [6]). *Let $\tilde{D}$, $\tilde{X}$, $Y \in \mathbb{C}^{n\times n}$ be given, $\tilde{D}$ be diagonal, $\tilde{\lambda}_i := \tilde{D}_{ii}$, $i = 1, \ldots, n$, $R := Y(A\tilde{X} - B\tilde{X}\tilde{D})$, and $S := I_n - YB\tilde{X}$. If $\|S\|_\infty < 1$, then B, $\tilde{X}$, and Y are nonsingular, and all the eigenvalues are included in $\bigcup_{i=1}^n \langle\tilde{\lambda}_i, \hat{r}_i\rangle$, where $\hat{r} := |R|\mathbb{1} + (\|R\|_\infty/(1 - \|S\|_\infty))|S|\mathbb{1}$.*

COROLLARY 3.2. *Let $\tilde{X}$, Y, $\tilde{\lambda}_i$, R, and S be as in Theorem 3.1, $t := |S|\mathbb{1}$ and $u := |R|\mathbb{1}$. If $\|t\|_\infty < 1$, then B, $\tilde{X}$, and Y are nonsingular, and all the eigenvalues are included in $\bigcup_{i=1}^n \langle\tilde{\lambda}_i, r_i\rangle$, where $r := u + \|u\|_t t$.*

Proof. Let $\tilde{D}$ be as in Theorem 3.1. Similarly to [6, proof of Theorem 3], $\|S\|_\infty = \|t\|_\infty < 1$ implies the nonsingularities of $I_n - S$, B, $\tilde{X}$, and Y, (1.1) is equivalent to the standard eigenvalue problem

$$(\tilde{D} + Q)y = \lambda y, \qquad Q := (I_n - S)^{-1}R, \quad y := \tilde{X}^{-1}x, \tag{3.1}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

and all the eigenvalues are included in $\bigcup_{i=1}^{n} \langle \tilde{\lambda}_i, (|Q|\mathbb{1})_i \rangle$. From Lemma 2.3, we have $|Q|\mathbb{1} \le |(I_n - S)^{-1}|u \le r$, showing the result. □

Remark 3.3. The eigenvalue inclusion comes from the Gershgorin theorem. If k of the disks form a connected domain which is isolated from the other disks, therefore, this domain contains precisely k eigenvalues.

LEMMA 3.4. *Let $\hat{r}$ and r be as in Theorem* 3.1 *and Corollary* 3.2*, respectively. Then $r \le \hat{r}$ holds.*

Proof. Let R and S be as in Theorem 3.1, and let t and u be as in Corollary 3.2. The inequality holds immediately from $\|u\|_t \le \|R\|_\infty/(1 - \|S\|_\infty)$. □

From the above, the algorithm in section 3.4 computes n disks containing all the eigenvalues based on Corollary 3.2.

3.2. Individual eigenvector. If one of the disks is isolated from the other disks, enclosing an individual eigenvector is possible with only $\mathcal{O}(n^2)$ operations.

THEOREM 3.5. *Let $\tilde{X}$, $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$, and R be as in Theorem* 3.1*, t and r be as in Corollary* 3.2*, $i \in \{1, \ldots, n\}$, and $I^{(i)} \in \mathbb{R}^{(n-1)\times n}$ and $J^{(i)} \in \mathbb{R}^{n\times(n-1)}$ be I_n without the ith row and column, respectively. Assume $\|t\|_\infty < 1$ and $\langle \tilde{\lambda}_i, r_i \rangle$ is isolated from the other disks, and define $\tilde{d} := (\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)^T$, $f := |\tilde{d} - \tilde{\lambda}_i \mathbb{1}| - r_i \mathbb{1}$, $v := |R|J^{(i)}\mathbb{1}$, $w := |R|e^{(i)}$, $g := (I^{(i)}(v + \|v\|_t t))./(I^{(i)} f)$, $h := (I^{(i)}(w + \|w\|_t t))./(I^{(i)} f)$, and $q := h + \|h\|_g g$. Then $\langle \tilde{\lambda}_i, r_i \rangle$ contains precisely one eigenvalue λ^* of* (1.1)*, geometric multiplicity of λ^* is one, and there exists an eigenvector x^* corresponding to λ^* satisfying $|x^* - \tilde{X}_{:i}| \le |\tilde{X}|J^{(i)} q$.*

Remark 3.6. The isolation of $\langle \tilde{\lambda}_i, r_i \rangle$ gives $I^{(i)} f > 0$ and $\|g\|_\infty < 1$ (see the proof), so that g, h, and $\|h\|_g$ can be defined.

Remark 3.7. Observe that the computation of $\overline{\mathrm{fl}}(|\tilde{X}|J^{(i)} q)$ involves only $\mathcal{O}(n^2)$ operations if $\overline{\mathrm{fl}}(|\tilde{X}|)$, $\overline{\mathrm{fl}}(|R|)$, and $\overline{\mathrm{fl}}(t)$ have already been obtained.

Proof. The equivalence of (1.1) and (3.1), the isolation of $\langle \tilde{\lambda}_i, r_i \rangle$, and Remark 3.3 show that $\langle \tilde{\lambda}_i, r_i \rangle$ contains precisely one eigenvalue λ^* in (1.1). Thus the algebraic multiplicity of λ^* is one, so that its geometric multiplicity is also one. Let y^* be an eigenvector corresponding to λ^* in (3.1) satisfying $y_i^* = 1$. If we put $x^* = \tilde{X} y^*$, then x^* is an eigenvector corresponding to λ^* in (1.1), and it holds that

$$x^* - \tilde{X}_{:i} = \tilde{X} y^* - \tilde{X} e^{(i)} = \tilde{X}(y^* - e^{(i)}) = \tilde{X}((e^{(i)} + J^{(i)} I^{(i)} y^*) - e^{(i)}) = \tilde{X} J^{(i)} I^{(i)} y^*,$$

which implies $|x^* - \tilde{X}_{:i}| \le |\tilde{X}|J^{(i)}|I^{(i)} y^*|$. We hence show $|I^{(i)} y^*| \le q$ for proving $|x^* - \tilde{X}_{:i}| \le |\tilde{X}|J^{(i)} q$.

Let $\tilde{D}$, u, and Q be as in Theorem 3.1, Corollary 3.2, and (3.1), respectively, $\underline{f} := (\tilde{\lambda}_1 - \lambda^*, \ldots, \tilde{\lambda}_n - \lambda^*)^T$, $Z_Q := I^{(i)}(\tilde{D} - \lambda^* I_n + Q)J^{(i)}$, and $Z := I^{(i)}(\tilde{D} - \lambda^* I_n)J^{(i)}$. The isolation of $\langle \tilde{\lambda}_i, r_i \rangle$ implies $\tilde{\lambda}_j \notin \langle \tilde{\lambda}_i, r_i \rangle$, $\forall j \in \{1, \ldots, n\} \setminus \{i\}$, so that $|\tilde{\lambda}_j - \tilde{\lambda}_i| - r_i > 0$, showing $I^{(i)} f > 0$. This isolation also gives $r_j + r_i < |\tilde{\lambda}_j - \tilde{\lambda}_i|$, showing $r_j/f_j < 1$. This and $v \le u$ yield $(v + \|v\|_t t)_j/f_j \le (u + \|u\|_t t)_j/f_j = r_j/f_j < 1$, which gives $\|g\|_\infty < 1$. Since $\lambda^* \in \langle \tilde{\lambda}_i, r_i \rangle$, $\tilde{\lambda}_j \notin \langle \tilde{\lambda}_i, r_i \rangle$, and $|\tilde{\lambda}_j - \tilde{\lambda}_i| - r_i > 0$, we have $|\tilde{\lambda}_j - \lambda^*| \ge |\tilde{\lambda}_j - \tilde{\lambda}_i| - r_i > 0$, so that $I^{(i)}|\underline{f}| \ge I^{(i)} f > 0$. The inequality $|\tilde{\lambda}_j - \lambda^*| > 0$ moreover gives the nonsingularity of Z. It holds that

$$I_{n-1} - Z^{-1} Z_Q = -Z^{-1} I^{(i)} Q J^{(i)} = -(I^{(i)} Q J^{(i)})./(I^{(i)} \underline{f} \mathbb{1}^T). \tag{3.2}$$

Let $\underline{g} := |I_{n-1} - Z^{-1} Z_Q|\mathbb{1}$. From (3.2) and Lemmas 2.3 and 2.5, we obtain

$$\underline{g} = ((I^{(i)}|Q|J^{(i)})./(I^{(i)}|\underline{f}|\mathbb{1}^T))\mathbb{1} = (I^{(i)}|(I_n - S)^{-1} R|J^{(i)}\mathbb{1})./(I^{(i)}|\underline{f}|) \le g. \tag{3.3}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

This, $\|g\|_\infty < 1$, and Lemma 2.1 give that Z_Q is nonsingular. From the definition of y^*, we have $(\tilde{D} - \lambda^* I_n + Q)y^* = 0$, which gives $I^{(i)}(\tilde{D} - \lambda^* I_n + Q)y^* = 0$. Since $y_i^* = 1$ and $I^{(i)} D^* e^{(i)} = 0$ for any diagonal matrix D^*, we obtain

$$\begin{aligned} I^{(i)}(\tilde{D} - \lambda^* I_n + Q)y^* = 0 &\Leftrightarrow I^{(i)}(\tilde{D} - \lambda^* I_n + Q)(e^{(i)} + J^{(i)} I^{(i)} y^*) = 0 \\ &\Leftrightarrow Z_Q I^{(i)} y^* = -I^{(i)}(\tilde{D} - \lambda^* I_n + Q)e^{(i)} \\ &\Leftrightarrow Z_Q I^{(i)} y^* = -I^{(i)} Q e^{(i)}. \end{aligned}$$

This and the nonsingularities of Z and Z_Q yield

$$\begin{aligned} I^{(i)} y^* &= -Z_Q^{-1} I^{(i)} Q e^{(i)} = -Z_Q^{-1} Z Z^{-1} I^{(i)} Q e^{(i)} \\ &= -(I_{n-1} - (I_{n-1} - Z^{-1} Z_Q))^{-1}((I^{(i)} Q e^{(i)})./(I^{(i)} \underline{f})). \end{aligned} \tag{3.4}$$

It follows from Lemma 2.3 that

$$|(I^{(i)} Q e^{(i)})./(I^{(i)} \underline{f})| = (I^{(i)} |(I_n - S)^{-1} R| e^{(i)})./(I^{(i)} |\underline{f}|) \le h. \tag{3.5}$$

From (3.3), (3.4), (3.5), $\|g\|_\infty < 1$, and Lemma 2.3, we finally obtain

$$|I^{(i)} y^*| \le |(I_{n-1} - (I_{n-1} - Z^{-1} Z_Q)^{-1}| h \le h + \|h\|_{\underline{g}} \underline{g} \le q. \qquad \square$$

3.3. Invariant subspace. When some of the disks are connected, we cannot apply Theorem 3.5 for these disks. Even in this case, the connected domain contains some eigenvalues, and we can enclose an invariant subspace corresponding to these eigenvalues. Let $\tilde{X}$, Y, $\tilde{\lambda}_1, \dots, \tilde{\lambda}_n$, and S be as in Theorem 3.1, $k \in \{1, \dots, n\}$, $1 \le i_1 < \cdots < i_k \le n$, and $\langle \tilde{\lambda}_{i_1}, r_{i_1} \rangle, \dots, \langle \tilde{\lambda}_{i_k}, r_{i_k} \rangle$ form a connected domain which is isolated from the other disks, and $\mathbf{v} := \{i_1, \dots, i_k\}$, $\mathbf{u} := \{1, \dots, n\} \setminus \mathbf{v}$, and U and V be the submatrix of I_n with columns $\mathbf{u}$ and $\mathbf{v}$, respectively. For $\tilde{\lambda} \in \mathbb{C}$, define the $n \times n$ diagonal matrix $\tilde{D}'$ such that

$$\tilde{D}'_{ii} = \begin{cases} \tilde{\lambda} & (i \in \mathbf{v}) \\ \tilde{\lambda}_i & (i \in \mathbf{u}) \end{cases}, \ i = 1, \dots, n.$$

In practical application, $\tilde{\lambda}$ is obtained such that $\tilde{\lambda} = \mathrm{fl}((\sum_{p=1}^{k} \tilde{\lambda}_{i_p})/k)$. Define $R' := Y(A\tilde{X} - B\tilde{X}\tilde{D}')$ and $Q' := (I_n - S)^{-1} R'$ if $I_n - S$ is nonsingular.

Remark 3.8. Let R be as in Theorem 3.1. Since $R' = R + YB\tilde{X}(\tilde{D} - \tilde{D}')$, R' can be enclosed with $\mathcal{O}(n^2)$ operations by reusing the enclosures of R and $YB\tilde{X}$.

As described in section 1, the eigenvalues and invariant subspace can be found by considering $AP_s = BP_s\Lambda$. If $I_n - S$ is nonsingular, this equality is equivalent to $(\tilde{D}' + Q')\hat{P} = \hat{P}\Lambda$, where $\hat{P} := \tilde{X}^{-1} P_s$. Namely, $\tilde{X}\hat{P}$ spans the invariant subspace in (1.1). In order to exploit the special structure of $\tilde{D}'$, we deal with $(\tilde{D}' + Q')\hat{P} = \hat{P}\Lambda$ instead of $AP_s = BP_s\Lambda$. The arbitrariness of $\hat{P}$ can be removed by freezing its k rows. We hence set $\hat{P}$ such that the $i_1, \dots, i_k$th rows of $\hat{P}$ coincide with those of V, i.e., $V^T\hat{P} = V^T V = I_k$. Similarly to [9], we correct the unknown quantities $U^T\hat{P}$ and Λ into $P \in \mathbb{C}^{n \times k}$, i.e., we consider finding P with $U^T\hat{P} = U^T P$ and $V^T P = \Lambda$. Since $UU^T + VV^T = I_n$, we have

$$\begin{aligned} (\tilde{D}' + Q')\hat{P} = \hat{P}\Lambda &\Leftrightarrow (\tilde{D}' + Q')(UU^T + VV^T)\hat{P} = (UU^T + VV^T)\hat{P}\Lambda \\ &\Leftrightarrow (\tilde{D}' + Q')(UU^T P + V) = (UU^T P + V)V^T P \\ &\Leftrightarrow ((\tilde{D}' + Q')UU^T - VV^T)P - UU^T P V^T P + (\tilde{D}' + Q')V = 0. \end{aligned}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Hence P can be obtained by solving $F(P) = 0$, where $F(P) := ((\tilde{D}' + Q')UU^T - VV^T)P - UU^TPV^TP + (\tilde{D}' + Q')V$. Observe that $F(\tilde{\lambda}V) \approx 0$ if $(\tilde{D}' + Q')V \approx \tilde{\lambda}V$, since $U^TV = 0$. The derivative $F'_P(H)$ can be written as $F'_P(H) = ((\tilde{D}' + Q')UU^T - VV^T - UU^TPV^T)H - UU^THV^TP$. We thus obtain $F'_{\tilde{\lambda}V}(H) = Z_QH$, where $Z_Q := (\tilde{D}' - \tilde{\lambda}I_n + Q')UU^T - VV^T$. If $F'_{\tilde{\lambda}V}(H)$ is invertible, we can define the Newton operator $N(P) := P - (F'_{\tilde{\lambda}V})^{-1}(F(P))$, and $N(P) = P$ is a fixed point equation for P. For enclosing P, we apply the Brouwer's fixed point theorem to $N(P)$.

We present Lemma 3.9 for verifying the invertibility of $F'_{\tilde{\lambda}V}(H)$. If it holds that $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\} \subseteq \mathrm{int}(\langle\tilde{\lambda}V, P_r\rangle)$, where $P_r \in \mathbb{R}^{n\times k}$ has positive components, the Brouwer theorem shows that the fixed point, i.e., the solution of $F(P) = 0$, exists in $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\}$. We verify this inclusion by computing the superset of $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\}$. The superset can be computed by the following idea: The equality $N(P) = P - (F'_{\tilde{\lambda}V})^{-1}(F(P))$ is equivalent to $F'_{\tilde{\lambda}V}(N(P)) = F'_{\tilde{\lambda}V}(P) - F(P)$, i.e., $Z_QN(P) = Z_QP - F(P)$. Hence $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\}$ is the set of all solutions of a parameterized matrix equation $Z_QN_P = Z_QP - F(P)$, where $N_P \in \mathbb{C}^{n\times k}$ is unknown and $P \in \langle\tilde{\lambda}V, P_r\rangle$ is the parameter. Therefore the superset can be obtained by enclosing the solution set. We establish Lemma 3.10 for obtaining the superset based on this idea and formulate and prove Theorem 3.11 for enclosing the eigenvalues and invariant subspace based on Lemmas 3.9 and 3.10. In practical application, we need to determine P_r satisfying the above inclusion. For $\overline{P}_\varepsilon \in \mathbb{R}^{n\times k}$ having positive components, let $\langle\tilde{\lambda}V, \overline{P}_\varepsilon\rangle$ be the superset of $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\}$. If $\overline{P}_\varepsilon < P_r$, the above inclusion is satisfied. Theorem 3.15 is presented for determining P_r based on this idea.

LEMMA 3.9. *Let* $\mathbf{v}$, $\mathbf{u}$, U, V, $\tilde{\lambda}$, R', *and* $F'_{\tilde{\lambda}V}(H)$ *be as above,* $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$ *be as in Theorem* 3.1, *and* t *be as in Corollary* 3.2. *Assume* $\tilde{\lambda}_i \neq \tilde{\lambda}$ $\forall i \in \mathbf{u}$ *and* $\|t\|_\infty < 1$. *Let* ϕ *be an n-vector satisfying*

$$\phi_i = \begin{cases} -1 & (i \in \mathbf{v}) \\ \tilde{\lambda}_i - \tilde{\lambda} & (i \in \mathbf{u}) \end{cases}, \quad i = 1, \ldots, n,$$

$\nu' := |R'|UU^T\mathbb{1}$, *and* $\mu := (\nu' + \|\nu'\|_t t)./|\phi|$. *If* $\|\mu\|_\infty < 1$, $F'_{\tilde{\lambda}V}(H)$ *is invertible.*

Proof. Let $\tilde{D}'$, Q', and Z_Q be as the above, and $Z := (\tilde{D}' - \tilde{\lambda}I_n)UU^T - VV^T$. We prove the nonsingularity of Z_Q using Lemma 2.1, since $F'_{\tilde{\lambda}V}(H)$ is invertible if Z_Q is nonsingular. From $\tilde{\lambda}_i \neq \tilde{\lambda}$ $\forall i \in \mathbf{u}$, Z is nonsingular. We have

$$I_n - Z^{-1}Z_Q = -Z^{-1}Q'UU^T = (-Q'UU^T)./(\phi\mathbb{1}^T).$$

This and Lemmas 2.3 and 2.5 yield

$$\begin{aligned} |I_n - Z^{-1}Z_Q|\mathbb{1} &= |(-Q'UU^T)./(\phi\mathbb{1}^T)|\mathbb{1} = (|Q'|UU^T./|\phi|\mathbb{1}^T)\mathbb{1} \\ &= (|Q'|UU^T\mathbb{1})./|\phi| \leq (|(I_n - S)^{-1}|\nu')./|\phi| \leq \mu, \end{aligned} \tag{3.6}$$

so that $\|\mu\|_\infty < 1$ and Lemma 2.1 shows the nonsingularity. ∎

LEMMA 3.10. *Let* U, V, $\tilde{\lambda}$, $N(P)$, R', P_r *be as above,* t *be as in Corollary* 3.2, *and* ϕ *and* μ *be as in Lemma* 3.9. *Assume all the conditions in Lemma* 3.9 *are satisfied and let* $w := (\|R'_{:i_1}\|_t, \ldots, \|R'_{:i_k}\|_t)^T$, $R_w \geq |R'|V + tw^T$, $T := (R_w + UU^TP_rV^TP_r)./(|\phi|\mathbb{1}^T)$, $z := (\|T_{:1}\|_\mu, \ldots, \|T_{:k}\|_\mu)^T$, *and* $P_\varepsilon := T + \mu z^T$. *Then* $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\} \subseteq \langle\tilde{\lambda}V, P_\varepsilon\rangle$ *holds.*

Proof. Let Q', $F(P)$, Z_Q, and N_P be as above, and let Z be as in the proof of Lemma 3.9. As described above, $\{N(P) : P \in \langle\tilde{\lambda}V, P_r\rangle\}$ is the set of all solutions

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

of $Z_Q N_P = Z_Q P - F(P)$, $P \in \langle \tilde{\lambda} V, P_r \rangle$. We hence prove that $\langle \tilde{\lambda} V, P_\varepsilon \rangle$ includes the solution set, i.e., $|\tilde{\lambda} V - N_P| \le P_\varepsilon$ holds for any $P \in \langle \tilde{\lambda} V, P_r \rangle$. Since all the conditions in Lemma 3.9 are satisfied, Z_Q is nonsingular. Any P can be written as $P = \tilde{\lambda} V + \underline{P}_r$, where $\underline{P}_r \in \mathbb{C}^{n \times k}$ satisfies $|\underline{P}_r| \le P_r$. It thus follows for any P that

$$\begin{aligned} Z_Q P - F(P) &= -(\tilde{D}' + Q')V - \tilde{\lambda} U U^T P + U U^T P V^T P \\ &= -(\tilde{D}' + Q')V - \tilde{\lambda} U U^T (\tilde{\lambda} V + \underline{P}_r) + U U^T (\tilde{\lambda} V + \underline{P}_r) V^T (\tilde{\lambda} V + \underline{P}_r) \\ &= -(\tilde{D}' + Q')V + U U^T \underline{P}_r V^T \underline{P}_r. \end{aligned}$$

Hence $Z_Q N_P = Z_Q P - F(P)$ is equivalent to $Z_Q N_P = -(\tilde{D}' + Q')V + U U^T \underline{P}_r V^T \underline{P}_r$, where $\underline{P}_r \in \langle 0, P_r \rangle$. This and $\tilde{D}' V = \tilde{\lambda} V$ give

$$\begin{aligned} \tilde{\lambda} V - N_P &= \tilde{\lambda} V - Z_Q^{-1}(-(\tilde{D}' + Q')V + U U^T \underline{P}_r V^T \underline{P}_r) \\ &= Z_Q^{-1}(Z_Q(\tilde{\lambda} V) + (\tilde{D}' + Q')V - U U^T \underline{P}_r V^T \underline{P}_r) \\ &= Z_Q^{-1}(Q'V - U U^T \underline{P}_r V^T \underline{P}_r) = Z_Q^{-1} Z Z^{-1}(Q'V - U U^T \underline{P}_r V^T \underline{P}_r) \\ &= (I_n - (I_n - Z^{-1} Z_Q))^{-1}((Q'V - U U^T \underline{P}_r V^T \underline{P}_r)./(\phi \mathbb{1}^T)). \end{aligned}$$

From this, (3.6), Corollary 2.4, and $|\underline{P}_r| \le P_r$, it holds for any $\underline{P}_r$, i.e., for any P, that

$$\begin{aligned} |\tilde{\lambda} V - N_P| &\le |(I_n - (I_n - Z^{-1} Z_Q))^{-1}||(Q'V - U U^T \underline{P}_r V^T \underline{P}_r)./(\phi \mathbb{1}^T)| \\ &\le |(I_n - (I_n - Z^{-1} Z_Q))^{-1}|((|Q'|V + U U^T |\underline{P}_r| V^T |\underline{P}_r|)./(|\phi| \mathbb{1}^T)) \\ &\le |(I_n - (I_n - Z^{-1} Z_Q))^{-1}|((|R'|V + t w^T + U U^T P_r V^T P_r)./(|\phi| \mathbb{1}^T)) \\ &\le |(I_n - (I_n - Z^{-1} Z_Q))^{-1}| T \le P_\varepsilon. \qquad \square \end{aligned}$$

THEOREM 3.11. *Let U, V, $\tilde{\lambda}$, and P_r be as above, $\tilde{X}$ be as in Theorem* 3.1*, P_ε be as in Lemma* 3.10*, and $\overline{P}_\varepsilon \ge P_\varepsilon$. If all the assumptions in Lemma* 3.9 *are true and $\overline{P}_\varepsilon < P_r$, then k eigenvalues are included in $\langle \tilde{\lambda}, \overline{\rho}(V^T \overline{P}_\varepsilon) \rangle$ and $\langle \tilde{X} V, |\tilde{X}| U U^T \overline{P}_\varepsilon \rangle$ contains a matrix which spans the corresponding invariant subspace in* (1.1).

Remark 3.12. The bound $\overline{\rho}(V^T \overline{P}_\varepsilon)$ can be computed similarly to [9, section 3].

Proof. Let $\hat{P}$, Λ, and $F(P)$ be as above. We prove $\Lambda \in \langle \tilde{\lambda} I_k, V^T \overline{P}_\varepsilon \rangle$ and $\tilde{X} \hat{P} \in \langle \tilde{X} V, |\tilde{X}| U U^T \overline{P}_\varepsilon \rangle$, since eigenvalues of Λ are those of (1.1), $\tilde{X} \hat{P}$ spans the corresponding invariant subspace in (1.1), and the discussion similar to [9, section 3] yields that $\langle \tilde{\lambda}, \overline{\rho}(V^T \overline{P}_\varepsilon) \rangle$ contains all eigenvalues of any matrix included in $\langle \tilde{\lambda} I_k, V^T \overline{P}_\varepsilon \rangle$. From the assumptions and Lemma 3.10, $\{N(P) : P \in \langle \tilde{\lambda} V, P_r \rangle\} \subseteq \langle \tilde{\lambda} V, \overline{P}_\varepsilon \rangle \subseteq \mathrm{int}(\langle \tilde{\lambda} V, P_r \rangle)$ holds. This and the Brouwer theorem yield that $\langle \tilde{\lambda} V, \overline{P}_\varepsilon \rangle$ contains P satisfying $F(P) = 0$, i.e., $U^T P = U^T \hat{P}$ and $V^T P = \Lambda$. This, $V^T \hat{P} = I_k$, and center-radius interval arithmetic evaluations (e.g., [16]) give

$$\begin{aligned} \Lambda &= V^T P \in V^T \langle \tilde{\lambda} V, \overline{P}_\varepsilon \rangle \subseteq \langle \tilde{\lambda} I_k, V^T \overline{P}_\varepsilon \rangle, \\ \tilde{X} \hat{P} &= \tilde{X}(U U^T + V V^T) \hat{P} = \tilde{X}(U U^T P + V) \\ &\in \tilde{X} U U^T \langle \tilde{\lambda} V, \overline{P}_\varepsilon \rangle + \tilde{X} V \subseteq \langle \tilde{X} V, |\tilde{X}| U U^T \overline{P}_\varepsilon \rangle. \qquad \square \end{aligned}$$

Remark 3.13. We can also utilize the Gershgorin theorem for enclosing all the eigenvalues of any matrix included in $\langle \tilde{\lambda} I_k, V^T \overline{P}_\varepsilon \rangle$. If $\overline{\rho}(V^T \overline{P}_\varepsilon)$ is close to $\rho(V^T \overline{P}_\varepsilon)$, however, this approach does not give an enclosure tighter than $\langle \tilde{\lambda}, \overline{\rho}(V^T \overline{P}_\varepsilon) \rangle$. The reason is as follows: The Gershgorin disks are included in $\bigcup_{i=1}^{k} \langle \tilde{\lambda}, ((V^T \overline{P}_\varepsilon) \mathbb{1})_i \rangle$. This

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

union contains $\langle\tilde{\lambda}, \rho(V^T\overline{P}_\varepsilon)\rangle$, since $\bigcup_{i=1}^k\langle\tilde{\lambda}, ((V^T\overline{P}_\varepsilon)\mathbb{1})_i\rangle = \langle\tilde{\lambda}, \max_i((V^T\overline{P}_\varepsilon)\mathbb{1})_i\rangle = \langle\tilde{\lambda}, \|V^T\overline{P}_\varepsilon\|_\infty\rangle \supseteq \langle\tilde{\lambda}, \rho(V^T\overline{P}_\varepsilon)\rangle$.

Remark 3.14. If $\langle\tilde{\lambda}, \overline{\rho}(V^T\overline{P}_\varepsilon)\rangle$ is isolated from $\bigcup_{i\in\mathbf{u}}\langle\tilde{\lambda}_i, r_i\rangle$, the k eigenvalues contained in $\langle\tilde{\lambda}, \overline{\rho}(V^T\overline{P}_\varepsilon)\rangle$ coincide with those in $\bigcup_{i\in\mathbf{v}}\langle\tilde{\lambda}_i, r_i\rangle$.

THEOREM 3.15. *Let U, V, and P_r be as above, R_w and P_ε be as in Lemma* 3.10*, $\underline{P}_\varepsilon^*$ be P_ε when $P_r = 0$, $\sigma, \eta \in \mathbb{F}$, $\underline{P}_\varepsilon \in \mathbb{F}^{n\times k}$, and $\overline{P}_\varepsilon := \mathrm{fl}_\triangle((1+\sigma\eta^2)\underline{P}_\varepsilon)$. Assume $\mathrm{fl}_\triangle(a \bullet b) = (1+\delta)(a\bullet b)$ for $a, b \in \mathbb{F}$, where $\bullet \in \{+, *\}$ and $|\delta| \le \mathtt{eps}$, $\underline{P}_\varepsilon \ge \underline{P}_\varepsilon^*$, $R_w > 0$, $\sigma \ge \|(UU^T\underline{P}_\varepsilon V^T\underline{P}_\varepsilon)./R_w\|_{\mathrm{M}}$, $\sigma(1+\mathtt{eps})^6 < 1/4$,*

$$\frac{2(1+\mathtt{eps})^2}{1+\sqrt{1-4\sigma(1+\mathtt{eps})^6}} < \eta < \frac{1+\sqrt{1-4\sigma(1+\mathtt{eps})^6}}{2\sigma(1+\mathtt{eps})^4}$$

and $P_r = \eta\underline{P}_\varepsilon$. Then $P_\varepsilon \le \overline{P}_\varepsilon < P_r$ follows.

Proof. We prove $P_\varepsilon \le \overline{P}_\varepsilon$ and $\overline{P}_\varepsilon < P_r$ under these assumptions. Let ϕ and T be as in Lemmas 3.9 and 3.10, respectively, and $\Phi := (VV^T\underline{P}_\varepsilon V^T\underline{P}_\varepsilon)./R_w$. From $\sigma \ge \|\Phi\|_{\mathrm{M}}$ and $P_r = \eta\underline{P}_\varepsilon$, we have

$$T{=}(R_w{+}\eta^2UU^T\underline{P}_\varepsilon V^T\underline{P}_\varepsilon)./(|\phi|\mathbb{1}^T){=}(R_w{+}\eta^2R_w\circ\Phi)./(|\phi|\mathbb{1}^T){\le}(1{+}\sigma\eta^2)R_w./(|\phi|\mathbb{1}^T),$$

which implies $P_\varepsilon \le (1+\sigma\eta^2)\underline{P}_\varepsilon^* \le (1+\sigma\eta^2)\underline{P}_\varepsilon$. The inequality $R_w > 0$ gives $\underline{P}_\varepsilon > 0$ and $\sigma > 0$. These and $\eta > 0$ yield $(1+\sigma\eta^2)\underline{P}_\varepsilon \le \overline{P}_\varepsilon$, so that $P_\varepsilon \le \overline{P}_\varepsilon$ holds. The assumption with respect to $\mathrm{fl}_\triangle(\cdot)$ shows $\overline{P}_\varepsilon = (1{+}\delta_4)(1{+}\delta_3)(1{+}\sigma\eta^2(1{+}\delta_1)(1{+}\delta_2))\underline{P}_\varepsilon$, where $|\delta_i| \le \mathtt{eps}$, $i = 1, \ldots, 4$, which yields $\overline{P}_\varepsilon \le (1+\mathtt{eps})^2(1+\sigma\eta^2(1+\mathtt{eps})^2)\underline{P}_\varepsilon$. The inequalities regarding to $\sigma(1+\mathtt{eps})^6$ and η moreover give $(1+\mathtt{eps})^2(1+\sigma\eta^2(1+\mathtt{eps})^2) < \eta$. These discussions prove $\overline{P}_\varepsilon < \eta\underline{P}_\varepsilon = P_r$. ∎

Remark 3.16. In the algorithm in section 3.4, $\overline{P}_\varepsilon$ and P_r are "determined" based on Theorem 3.15, but P_r and P_ε are not "numerically computed," and only $\overline{P}_\varepsilon$ is computed. Note that $P_\varepsilon \le \overline{P}_\varepsilon < P_r$ is still valid even in this case, and computing only $\overline{P}_\varepsilon$ is sufficient for numerically enclosing the eigenvalues and invariant subspace based on Theorem 3.11. The algorithm in section 4 is designed similarly.

3.4. Proposed algorithm.

Based on the theories in sections 3.1, 3.2, and 3.3, we propose the algorithm which encloses all the eigenvalues and invariant subspaces.

ALGORITHM 1. *Let $\tilde{D}$, $\tilde{X}$, $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$, Y, R, t, r, $J^{(i)}$, and q be as in this section. This algorithm encloses all the eigenvalues and invariant subspaces based on the theories in sections* 3.1, 3.2, *and* 3.3.

Step 1. *Compute $\tilde{D}$ and $\tilde{X}$ by the numerical GED of A and B.*

Step 2. *Compute $Y = \mathrm{fl}((B\tilde{X})^{-1})$, $\overline{\mathrm{fl}}(|R|)$, and $\overline{\mathrm{fl}}(t)$. If $\overline{\mathrm{fl}}(\|t\|_\infty) \ge 1$, terminate with failure.*

Step 3. *Compute $\overline{\mathrm{fl}}(r)$ and initialize the list $\mathcal{L}$ such that $\mathcal{L} = \{1, \ldots, n\}$.*

Step 4. *If $\mathcal{L}$ is empty, terminate. Otherwise let i be the smallest integer in $\mathcal{L}$.*

Step 5. *If $\langle\tilde{\lambda}_i, \overline{\mathrm{fl}}(r_i)\rangle$ is isolated from the other disks, delete i from $\mathcal{L}$, and enclose an individual eigenvector corresponding to the eigenvalue included in $\langle\tilde{\lambda}_i, \overline{\mathrm{fl}}(r_i)\rangle$ by computing $\overline{\mathrm{fl}}(|\tilde{X}|J^{(i)}q)$. Otherwise let $\bigcup_{j=1}^k\langle\tilde{\lambda}_{i_j}, \overline{\mathrm{fl}}(r_{i_j})\rangle$, where $i \in \{i_1, \ldots, i_k\} \subseteq \mathcal{L}$, be the connected disks which are isolated from the other disks, delete $i_1, \ldots, i_k$ from $\mathcal{L}$, and enclose the k eigenvalues and corresponding invariant subspace by Algorithm* 2. *Go back to Step* 4.

ALGORITHM 2. *Let $i_1, \ldots, i_k$, $\mathbf{u}$, $\tilde{\lambda}$, R', V, U, μ, w, R_w, $\underline{P}_\varepsilon^*$, $\underline{P}_\varepsilon$, $\overline{P}_\varepsilon$, σ, and η be as in section* 3.3, *and assume $\mathrm{fl}_\triangle(\cdot)$ satisfies the condition in Theorem* 3.15. *This algorithm encloses the k eigenvalues and corresponding invariant subspace based on the theories in section* 3.3.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Step 1. *Obtain* $\tilde{\lambda}$ *such that* $\tilde{\lambda} = \mathrm{fl}((\sum_{p=1}^{k} \tilde{\lambda}_{i_p})/k)$. *If* $\tilde{\lambda} \neq \tilde{\lambda}_j \ \forall j \in \mathbf{u}$ *cannot be verified, terminate with failure.*
Step 2. *Compute* $\overline{\mathrm{fl}}(\mu)$. *If* $\overline{\mathrm{fl}}(\|\mu\|_\infty) \geq 1$, *terminate with failure.*
Step 3. *Obtain* R_w *such that* $R_w = \overline{\mathrm{fl}}(|R'|V + tw^T)$. *If* $R_{w_{jp}} < \sqrt{\texttt{realmin}}$ *for* $j \in \{1, \dots, n\}$ *and* $p \in \{1, \dots, k\}$, *update* $R_{w_{jp}}$ *such that* $R_{w_{jp}} = \sqrt{\texttt{realmin}}$ *for all pairs of* j *and* p *satisfying this inequality.*
Step 4. *Compute* $\underline{P}_\varepsilon = \overline{\mathrm{fl}}(\underline{P}_\varepsilon^*)$ *and* $\sigma = \overline{\mathrm{fl}}(\|(UU^T \underline{P}_\varepsilon V^T \underline{P}_\varepsilon)./R_w\|_{\mathrm{M}})$. *If* $\overline{\mathrm{fl}}(\sigma(1 + \texttt{eps})^6) \geq 1/4$, *terminate with failure.*
Step 5. *Let* $\eta = \overline{\mathrm{fl}}(2(1+\texttt{eps})^3/(1+\sqrt{1-4\sigma(1+\texttt{eps})^6}))$. *If* $\eta < (1+\sqrt{1-4\sigma(1+\texttt{eps})^6})/(2\sigma(1+\texttt{eps})^4)$ *cannot be verified, terminate with failure.*
Step 6. *Compute* $\overline{P}_\varepsilon = \mathrm{fl}_\triangle((1 + \sigma\eta^2)\underline{P}_\varepsilon)$, $\overline{\mathrm{fl}}(|\tilde{X}|UU^T \overline{P}_\varepsilon)$, *and* $\overline{\rho}(\overline{\mathrm{fl}}(V^T \overline{P}_\varepsilon))$. *If* $\langle \tilde{\lambda}, \overline{\rho}(\overline{\mathrm{fl}}(V^T \overline{P}_\varepsilon)) \rangle \cap \bigcup_{i \in \mathbf{u}} \langle \tilde{\lambda}_i, \overline{\mathrm{fl}}(r_i) \rangle \neq \emptyset$, *terminate with failure.*
Step 7. *Terminate.*

Remark 3.17. The inequality $\min_{j,p} R_{w_{jp}} \geq \sqrt{\texttt{realmin}}$ implies $\min_{j,p} \underline{P}_{\varepsilon_{jp}} \geq \sqrt{\texttt{realmin}}$ and $\sigma \geq \sqrt{\texttt{realmin}}$. These and $\eta \geq 1$ show that underflow does not occur during the computation of $\overline{P}_\varepsilon$, so that $\mathrm{fl}_\triangle(\cdot)$ strictly satisfies the condition in Theorem 3.15 during this computation. Algorithms 4 and 5 have the similar property.

Remark 3.18. If Algorithm 1 terminated without failure, it is guaranteed that the obtained disks do not contain common eigenvalues, i.e., the union of these disks encloses all the eigenvalues.

In Algorithm 2, the computation of σ and $\overline{\mathrm{fl}}(|\tilde{X}|UU^T \overline{P}_\varepsilon)$ involve $\mathcal{O}(nk^2)$ and $\mathcal{O}(n^2k)$ operations, respectively. That of $\overline{\rho}(\overline{\mathrm{fl}}(V^T \overline{P}_\varepsilon))$ involves at most $\mathcal{O}(k^3)$ operations. The computational costs of the other parts are $\mathcal{O}(n^2)$. Hence Algorithm 2 involve $\mathcal{O}(n^2k + nk^2 + k^3)$ operations.

In Algorithm 1, the computations of $\tilde{D}$, $\tilde{X}$, Y, $\overline{\mathrm{fl}}(|R|)$, and $\overline{\mathrm{fl}}(t)$ require $\mathcal{O}(n^3)$ operations. That of $\overline{\mathrm{fl}}(|\tilde{X}|J^{(i)}q)$ requires $\mathcal{O}(n^2)$ operations for one isolated disk. If the number of isolated disks is j, therefore, enclosures of the j eigenvectors involve $\mathcal{O}(n^2j)$ operations. If the numbers of the connected domain and the disks contained in the each domain are m and $k_1, \dots, k_m$, respectively, then the m times executions of Algorithm 2 require $\mathcal{O}(n^2 \sum_{p=1}^{m} k_p + n \sum_{p=1}^{m} k_p^2 + \sum_{p=1}^{m} k_p^3)$ operations. Since $j + \sum_{p=1}^{m} k_p = n$, $\sum_{p=1}^{m} k_p^2 < (\sum_{p=1}^{m} k_p)^2 \leq n^2$, and $\sum_{p=1}^{m} k_p^3 < (\sum_{p=1}^{m} k_p)^3 \leq n^3$, Algorithm 1 involves only $\mathcal{O}(n^3)$ operations.

4. Enclosure utilizing BD. Let $\tilde{X}$ and t be as in section 3. When (1.1) has defective eigenvalues, $\tilde{X}$ becomes singular or ill conditioned, so that we cannot verify $\|t\|_\infty < 1$ and Algorithm 1 fails. Even in such situations, we can utilize the BD $X^{-1}(B^{-1}A)X = D$, where $X \in \mathbb{C}^{n \times n}$ is nonsingular and D is *block* diagonal with each diagonal block being upper triangular. In the BD, multiple or nearly multiple eigenvalues are gathered in the same diagonal block.

Remark 4.1. The BD in [12] computes *quasi*-triangular blocks, which contain real 2×2 diagonal subblocks for any pair of conjugate complex eigenvalues. Therefore the BD discussed here is slightly different from that in [12]. Similarly to the BD in [12], however, the BD discussed here can be achieved by executing Schur decomposition and repeatedly solving Sylvester equations. See the appendix for practical implementation.

In this section, we develop a theory for enclosing all the eigenvalues and invariant subspaces based on the BD. Let $\tilde{D}$ and $\tilde{X}$ be the approximations of D and X in the BD, respectively. Then $\tilde{D}$ can be written as $\tilde{D} = \mathrm{diag}(\tilde{D}^{(1)}, \dots, \tilde{D}^{(m)})$, where $\tilde{D}^{(i)}$, $i = 1, \dots, m$, are $n_i \times n_i$ upper triangular matrices with $\sum_{i=1}^{m} n_i = n$. We establish

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

theories for enclosing eigenvalues and individual eigenvectors when $n_i = 1$ and eigenvalues and invariant subspaces when $n_i \geq 2$ in sections 4.1 and 4.2, respectively. The algorithm based on these theories is proposed in section 4.3.

Let $i_1, \dots, i_k$ and $j_1, \dots, j_{m-k}$ be integers satisfying $1 \leq i_1 < \cdots < i_k \leq m$ and $n_{i_1} = \cdots = n_{i_k} = 1$, and $1 \leq j_1 < \cdots < j_{m-k} \leq m$ and $n_{j_p} \geq 2$, $p = 1, \dots, m-k$, respectively. We then have $\{i_1, \dots, i_k\} \cup \{j_1, \dots, j_{m-k}\} = \{1, \dots, m\}$. For $p = 1, \dots, m-k$, update $\tilde{D}^{(j_p)}$ such that $\tilde{D}^{(j_p)}_{qq} = \tilde{\lambda}_{j_p}$, $q = 1, \dots, n_{j_p}$, where $\tilde{\lambda}_{j_p} \in \mathbb{C}$. In practical application, $\tilde{\lambda}_{j_p}$ is obtained such that $\tilde{\lambda}_{j_p} = \mathrm{fl}((\sum_{q=1}^{n_{j_p}} \tilde{D}^{(j_p)}_{qq})/n_{j_p})$. Then $\tilde{D}$ is also updated. For $\tilde{D}$ and $\tilde{X}$ in this section, we define R, S, and t similarly to section 3. If $I_n - S$ is nonsingular, we also define Q similarly to section 3.

4.1. Block size one. Let $p \in \{i_1, \dots, i_k\}$, $\tilde{\lambda} := \tilde{D}^{(p)}$, $i := \sum_{q=1}^{p-1} n_q + 1$, $\mathbf{u} := \{1, \dots, n\} \backslash \{i\}$, and U be the submatrix of I_n with columns $\mathbf{u}$. If $I_n - S$ is nonsingular, discussion similar to (3.1) gives that (1.1) is equivalent to $(\tilde{D} + Q)\hat{y} = \lambda\hat{y}$, where $\hat{y} := \tilde{X}^{-1}x$. Namely, λ and $\tilde{X}\hat{y}$ are the eigenvalue and corresponding eigenvector in (1.1), respectively. For exploiting the structure of $\tilde{D}$, we treat this equality instead of (1.1). Analogously to section 3.3, we set $\hat{y}_i = 1$ and consider finding y satisfying $U^T\hat{y} = U^Ty$ and $y_i = \lambda$. Since $UU^T + e^{(i)}{e^{(i)}}^T = I_n$ and $\lambda = y_i = {e^{(i)}}^T y$, we obtain

$$\begin{aligned}(\tilde{D} + Q)\hat{y} = \lambda\hat{y} &\Leftrightarrow (\tilde{D} + Q)(UU^T + e^{(i)}{e^{(i)}}^T)\hat{y} = ({e^{(i)}}^T y)(UU^T + e^{(i)}{e^{(i)}}^T)\hat{y} \\ &\Leftrightarrow (\tilde{D} + Q)UU^Ty + (\tilde{D} + Q)e^{(i)} = ({e^{(i)}}^T y)UU^Ty + ({e^{(i)}}^T y)e^{(i)} \\ &\Leftrightarrow ((\tilde{D} + Q)UU^T - e^{(i)}{e^{(i)}}^T)y - UU^Ty{e^{(i)}}^T y + (\tilde{D} + Q)e^{(i)} = 0.\end{aligned}$$

Thus y can be obtained by solving $F(y) = 0$, where $F(y) := ((\tilde{D} + Q)UU^T - e^{(i)}{e^{(i)}}^T)y - UU^Ty{e^{(i)}}^T y + (\tilde{D} + Q)e^{(i)}$. Observe that $F(\tilde{\lambda}e^{(i)}) \approx 0$ if $(\tilde{D}+Q)e^{(i)} \approx \tilde{\lambda}e^{(i)}$. Moreover $F'_y(h)$ can be written as $F'_y(h) = ((\tilde{D} + Q)UU^T - e^{(i)}{e^{(i)}}^T - UU^Ty{e^{(i)}}^T)h - UU^Th{e^{(i)}}^T y$, so that $F'_{\tilde{\lambda}e^{(i)}}(h) = \mathsf{P}h$, where $\mathsf{P} := (\tilde{D} - \tilde{\lambda}I_n + Q)UU^T - e^{(i)}{e^{(i)}}^T$. For enclosing y, we apply the Brouwer theorem to $N(y)$, where $N(y) := y - (F'_{\tilde{\lambda}e^{(i)}})^{-1}(F(y))$, since $N(y) = y$ is a fixed point equation for y.

We present Lemmas 4.2 and 4.4 for verifying the invertibility of $F'_{\tilde{\lambda}e^{(i)}}(h)$ and obtaining the superset of $\{N(y) : y \in \langle\tilde{\lambda}e^{(i)}, y_r\rangle\}$, where $y_r \in \mathbb{R}^n$ has positive components, based on the idea analogous to that in section 3.3, respectively. Theorem 4.5 and Corollary 4.6 are established for enclosing the eigenvalue and eigenvector based on these lemmas and determining y_r based on the idea similar to that in section 3.3, respectively.

Lemma 4.2. *Let $\tilde{D}$, R, t, $\tilde{\lambda}$, U, and $F'_{\tilde{\lambda}e^{(i)}}(h)$ be as the above, $T \in \mathbb{C}^{n\times n}$, $W := I_n - T((\tilde{D} - \tilde{\lambda}I_n)UU^T - e^{(i)}{e^{(i)}}^T)$, and $\nu := |R|UU^T\mathbb{1}$. Assume $\|t\|_\infty < 1$ and define $\tau := |W|\mathbb{1} + |T|(\nu + \|\nu\|_t t)$. If $\|\tau\|_\infty < 1$, $F'_{\tilde{\lambda}e^{(i)}}(h)$ is invertible.*

Remark 4.3. In practical application, T is obtained such that $T = \mathrm{fl}(((\tilde{D} - \tilde{\lambda}I_n)UU^T - e^{(i)}{e^{(i)}}^T)^{-1})$. Then $(\tilde{D} - \tilde{\lambda}I_n)UU^T - e^{(i)}{e^{(i)}}^T$ and T are also block diagonal having nonzero structures similar to $\tilde{D}$. Hence the computation of T and the matrix multiplication within W require $\mathcal{O}(\sum_{p=1}^{m-k} n_{j_p}^3)$ operations.

Proof. Let S and P be as above. We prove the nonsingularity of P using Lemma 2.1, since $F'_{\tilde{\lambda}e^{(i)}}(h)$ is invertible if P is nonsingular. We have $I_n - T\mathsf{P} = W - TQUU^T$, so that $\|t\|_\infty < 1$ and Lemma 2.3 yield $|I_n - T\mathsf{P}|\mathbb{1} \leq |W|\mathbb{1} + |T||(I_n - S)^{-1}||R|UU^T\mathbb{1} \leq \tau$. This, $\|\tau\|_\infty < 1$ and Lemma 2.1 show the nonsingularity. ∎

Lemma 4.4. *Let R, t, U, $\tilde{\lambda}$, y_r, and $N(y)$ be as above, T and τ be as in Lemma 4.2, and $w := |R|e^{(i)}$. Assume $\|t\|_\infty < 1$ and $\|\tau\|_\infty < 1$, and let*

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

$\overline{w} \geq w + \|w\|_t t$, $v := |T|(\overline{w} + UU^T y_r e^{(i)^T} y_r)$, and $\xi := v + \|v\|_\tau \tau$. Then $\{N(y) : y \in \langle \tilde{\lambda} e^{(i)}, y_r\rangle\} \subseteq \langle \tilde{\lambda} e^{(i)}, \xi\rangle$ holds.

Proof. Let $\tilde{D}$, Q, $F(y)$, $F'_{\tilde{\lambda}e^{(i)}}(h)$, and P be as above. Analogously to section 3.3, we derive parameterized linear systems equivalent to $N(y) = y - (F'_{\tilde{\lambda}e^{(i)}})^{-1}(F(y))$ and show that $\langle \tilde{\lambda} e^{(i)}, \xi\rangle$ includes the solution set of the linear systems. From the assumptions and Lemma 4.2, P and T are nonsingular. We have

$$N(y) = y - (F'_{\tilde{\lambda}e^{(i)}})^{-1}(F(y)) \Leftrightarrow F'_{\tilde{\lambda}e^{(i)}}(N(y)) = F'_{\tilde{\lambda}e^{(i)}}(y) - F(y) \Leftrightarrow \mathsf{P}N(y) = \mathsf{P}y - F(y)$$
$$\Leftrightarrow \mathsf{P}N(y) = -\tilde{\lambda} UU^T y + UU^T y e^{(i)^T} y - (\tilde{D} + Q)e^{(i)}.$$

Thus the parameterized linear systems are

$$\mathsf{P}n_y = -\tilde{\lambda}UU^T y + UU^T y e^{(i)^T} y - (\tilde{D}+Q)e^{(i)}, \tag{4.1}$$

where $n_y \in \mathbb{C}^n$ is unknown and $y \in \langle \tilde{\lambda} e^{(i)}, y_r\rangle$ is the parameter. We hence prove $|\tilde{\lambda} e^{(i)} - n_y| \leq \xi$ for any y. Any $y \in \langle \tilde{\lambda} e^{(i)}, y_r\rangle$ can be written as $y = \tilde{\lambda} e^{(i)} + \underline{y}_r$, where $\underline{y}_r \in \mathbb{C}^n$ satisfies $|\underline{y}_r| \leq y_r$. From this and $U^T e^{(i)} = 0$, we have

$$\begin{aligned} &-\tilde{\lambda}UU^T y + UU^T y e^{(i)^T} y - (\tilde{D}+Q)e^{(i)} \\ &= -\tilde{\lambda}UU^T(\tilde{\lambda}e^{(i)} + \underline{y}_r) + UU^T(\tilde{\lambda}e^{(i)} + \underline{y}_r)e^{(i)^T}(\tilde{\lambda}e^{(i)} + \underline{y}_r) - (\tilde{D}+Q)e^{(i)} \\ &= -(\tilde{D}+Q)e^{(i)} + UU^T \underline{y}_r e^{(i)^T} \underline{y}_r, \end{aligned}$$

so that (4.1) is equivalent to $\mathsf{P}n_y = -(\tilde{D}+Q)e^{(i)} + UU^T\underline{y}_r e^{(i)^T}\underline{y}_r$, where $\underline{y}_r \in \langle 0, y_r\rangle$. This and $\tilde{D}e^{(i)} = \tilde{\lambda}e^{(i)}$ give

$$\begin{aligned} \tilde{\lambda}e^{(i)} - n_y &= \tilde{\lambda}e^{(i)} - \mathsf{P}^{-1}(-(\tilde{D}+Q)e^{(i)} + UU^T\underline{y}_r e^{(i)^T}\underline{y}_r) \\ &= \mathsf{P}^{-1}(\tilde{\lambda}\mathsf{P}e^{(i)} + (\tilde{D}+Q)e^{(i)} - UU^T\underline{y}_r e^{(i)^T}\underline{y}_r) \\ &= \mathsf{P}^{-1}(Qe^{(i)} - UU^T\underline{y}_r e^{(i)^T}\underline{y}_r) = \mathsf{P}^{-1}T^{-1}T(Qe^{(i)} - UU^T\underline{y}_r e^{(i)^T}\underline{y}_r) \\ &= (I_n - (I_n - T\mathsf{P}))^{-1}T(Qe^{(i)} - UU^T\underline{y}_r e^{(i)^T}\underline{y}_r) \end{aligned}$$

for any $\underline{y}_r$, i.e., for any y, so that $|I_n - T\mathsf{P}|\mathbb{1} \leq \tau$, $|\underline{y}_r| \leq y_r$, and Lemma 2.3 yield

$$\begin{aligned} |\tilde{\lambda}e^{(i)} - n_y| &\leq |(I_n - (I_n - T\mathsf{P}))^{-1}||T|(|(I_n - S)^{-1}||R|e^{(i)} + UU^T|\underline{y}_r|e^{(i)^T}|\underline{y}_r|) \\ &\leq |(I_n - (I_n - T\mathsf{P}))^{-1}||T|(\overline{w} + UU^T y_r e^{(i)^T} y_r) = |(I_n - (I_n - T\mathsf{P}))^{-1}|v \\ &\leq v + \|v\|_{|I_n - T\mathsf{P}|\mathbb{1}}|I_n - T\mathsf{P}|\mathbb{1} \leq v + \|v\|_\tau \tau = \xi. \qquad \square \end{aligned}$$

THEOREM 4.5. *Let i, $\tilde{X}$, $\tilde{\lambda}$, U, and y_r be as above, ξ be as in Lemma 4.4, and $\overline{\xi} \geq \xi$. If all the assumptions in Lemma 4.2 are true and $\overline{\xi} < y_r$, then an eigenvalue in (1.1) is included in $\langle \tilde{\lambda}, \overline{\xi}_i\rangle$, and $\langle \tilde{X}_{:i}, |\tilde{X}|UU^T\overline{\xi}\rangle$ contains an eigenvector corresponding to the included eigenvalue.*

Proof. Let $\hat{y}$, λ, and y be as above. We prove $\lambda \in \langle \tilde{\lambda}, \overline{\xi}_i\rangle$ and $\tilde{X}\hat{y} \in \langle \tilde{X}_{:i}, |\tilde{X}|UU^T\overline{\xi}\rangle$, since λ and $\tilde{X}\hat{y}$ are the eigenvalue and corresponding eigenvector in (1.1), respectively. From $\overline{\xi} < y_r$ and the Brouwer theorem, $y \in \langle \tilde{\lambda}e^{(i)}, \overline{\xi}\rangle$ holds. From this, $U^T\hat{y} = U^T y$, $e^{(i)^T}\hat{y} = \hat{y}_i = 1$, and $U^T e^{(i)} = 0$, we obtain

$$\begin{aligned} \lambda = y_i = e^{(i)^T} y \in e^{(i)^T}\langle \tilde{\lambda}e^{(i)}, \overline{\xi}\rangle &\subseteq \langle \tilde{\lambda}, e^{(i)^T}\overline{\xi}\rangle = \langle \tilde{\lambda}, \overline{\xi}_i\rangle, \\ \tilde{X}\hat{y} = \tilde{X}(UU^T + e^{(i)}e^{(i)^T})\hat{y} &= \tilde{X}UU^T y + \tilde{X}e^{(i)} \\ &\in \tilde{X}UU^T\langle \tilde{\lambda}e^{(i)}, \overline{\xi}\rangle + \tilde{X}_{:i} \subseteq \langle \tilde{X}_{:i}, |\tilde{X}|UU^T\overline{\xi}\rangle. \qquad \square \end{aligned}$$

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

COROLLARY 4.6. *Let U be as above, $\overline{w}$ and ξ be as in Lemma 4.4, $\underline{\xi}^*$ be ξ when $y_r = 0$, $\sigma, \eta \in \mathbb{F}$, $\underline{\xi} \in \mathbb{F}^n$, and $\overline{\xi} := \mathrm{fl}_\triangle((1+\sigma\eta^2)\underline{\xi})$. Assume $\underline{\xi} \geq \underline{\xi}^*$, $\overline{w} > 0$, $\sigma \geq \|(UU^T\underline{\xi}e^{(i)^T}\underline{\xi})./\overline{w}\|_\infty$, $y_r = \eta\underline{\xi}$, and $\mathrm{fl}_\triangle(\cdot)$, $\sigma(1+\mathtt{eps})^6$ and η satisfy the conditions in Theorem 3.15. Then $\xi \leq \overline{\xi} < y_r$ holds.*

Proof. The analogy of the proof of Theorem 3.15 shows the result. ∎

4.2. Block sizes two or more. Let $j \in \{j_1, \ldots, j_{m-k}\}$, so that $n_j \geq 2$. Let also $\tilde{\lambda} = \tilde{\lambda}_j$, $\mathbf{v} := \{\sum_{p=1}^{j-1} n_p + 1, \ldots, \sum_{p=1}^{j} n_p\}$, $\mathbf{u} := \{1, \ldots, n\} \setminus \mathbf{v}$, and let U and V be the submatrix of I_n with columns $\mathbf{u}$ and $\mathbf{v}$, respectively. Then $\tilde{D}^{(j)}_{11} = \cdots = \tilde{D}^{(j)}_{n_j n_j} = \tilde{\lambda}$ holds from the update in the beginning of this section. Similarly to section 3.3, we consider $AP_s = BP_s\Lambda$ for $P_s \in \mathbb{C}^{n \times n_j}$ and $\Lambda \in \mathbb{C}^{n_j \times n_j}$ to find the eigenvalues and invariant subspace, suppose the nonsingularity of $I_n - S$, deal with the equivalent problem $(\tilde{D}+Q)\hat{P} = \hat{P}\Lambda$, where $\hat{P} := \tilde{X}^{-1}P_s$, instead of $AP_s = BP_s\Lambda$, and set $V^T\hat{P} = I_{n_j}$. Our aim is to obtain P which satisfies $U^T\hat{P} = U^TP$ and $V^TP = \Lambda$ by solving $F(P) = 0$, where $F(P) := ((\tilde{D}+Q)UU^T - VV^T)P - UU^TPV^TP + (\tilde{D}+Q)V$. Observe that an approximation of P in this case is $V\tilde{D}^{(j)}$ if $(\tilde{D}+Q)V \approx V\tilde{D}^{(j)}$, so we utilize the derivative $F'_{V\tilde{D}^{(j)}}(H) = ((\tilde{D}+Q)UU^T - VV^T)H - UU^TH\tilde{D}^{(j)}$ and enclose P by using a fixed point equation $N(P) = P$, where $N(P) := P - (F'_{V\tilde{D}^{(j)}})^{-1}(F(P))$, and the Brouwer theorem.

We present theories for verifying the invertibility of $F'_{V\tilde{D}^{(j)}}(H)$, obtaining the superset of $\{N(P) : P \in \langle V\tilde{D}^{(j)}, P_r\rangle\}$, where $P_r \in \mathbb{R}^{n \times n_j}$ has positive components, based on the analogous idea, enclosing the eigenvalues and invariant subspace, and determining P_r based on the similar idea.

LEMMA 4.7. *Let $\tilde{D}$, $\tilde{D}^{(j)}$, $\tilde{\lambda}$, Q, t, U, V, and $F'_{V\tilde{D}^{(j)}}(H)$ be as above, $Z_Q := (\tilde{D} - \tilde{\lambda}I_n + Q)UU^T - VV^T$, $Z := (\tilde{D} - \tilde{\lambda}I_n)UU^T - VV^T$, $T \in \mathbb{C}^{n \times n}$, $W := I_n - TZ$, and ν and τ be as in Lemma 4.2. If $\|t\|_\infty < 1$ and $\|\tau\|_\infty < 1$, then Z_Q and T are nonsingular, and $F'_{V\tilde{D}^{(j)}}(H)$ is invertible.*

Proof. From Lemma 2.2, we obtain $\mathrm{vec}(F'_{V\tilde{D}^{(j)}}(H)) = \mathsf{P}\mathrm{vec}(H)$, where $\mathsf{P} := I_{n_j} \otimes ((\tilde{D}+Q)UU^T - VV^T) - \tilde{D}^{(j)^T} \otimes UU^T$. We prove the nonsingularity of Z_Q and T using Lemma 2.1 and show that the nonsingularity of Z_Q yields the nonsingularity of P since $F'_{V\tilde{D}^{(j)}}(H)$ is invertible if P is nonsingular.

We have $I_n - TZ_Q = W - TQUU^T$. This and Lemma 2.3 yield $|I_n - TZ_Q|\mathbb{1} \leq |W|\mathbb{1} + |T||Q|UU^T\mathbb{1} \leq \tau$. From this, $\|\tau\|_\infty < 1$ and Lemma 2.1, Z_Q and T are nonsingular. It moreover follows that

$$\mathsf{P} = \begin{pmatrix} (\tilde{D}+Q)UU^T - VV^T - \tilde{\lambda}UU^T & & \\ \vdots & \ddots & \\ -\tilde{D}^{(j)}_{1n_j}UU^T & \cdots & (\tilde{D}+Q)UU^T - VV^T - \tilde{\lambda}UU^T \end{pmatrix}$$

$$= \begin{pmatrix} Z_Q & & \\ \vdots & \ddots & \\ -\tilde{D}^{(j)}_{1n_j}UU^T & \cdots & Z_Q \end{pmatrix}. \tag{4.2}$$

This and the nonsingularity of Z_Q show the nonsingularity of P. ∎

LEMMA 4.8. *Let $\tilde{D}^{(j)}$, $\tilde{\lambda}$, R, t, U, V, $N(P)$, and P_r be as above, τ be as in Lemma 4.2, and T be as in Lemma 4.7. Assume $\|t\|_\infty < 1$ and $\|\tau\|_\infty < 1$, and let $w := (\|RV_{:1}\|_t, \ldots, \|RV_{:n_j}\|_t)^T$, $R_w \geq |R|V + tw^T$, $t_Q := (\|T_{:1}\|_\tau, \ldots, \|T_{:n}\|_\tau)^T$, $\overline{T} := |T| +$*

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

τt_Q^T, $\Delta := \tilde{D}^{(j)} - \tilde{\lambda} I_{n_j}$, $R_P := R_w + UU^T P_r V^T P_r$, *and* $P_\varepsilon := \sum_{p=0}^{n_j-1} (\overline{T} UU^T)^p \overline{T} R_P |\Delta|^p$. *Then* $\{N(P) : P \in \langle V\tilde{D}^{(j)}, P_r\rangle\} \subseteq \langle V\tilde{D}^{(j)}, P_\varepsilon\rangle$ *holds.*

Proof. Let $F(P)$ and $F'_{V\tilde{D}^{(j)}}(H)$ be as above, Z_Q be as in Lemma 4.7, and P be as in the proof of Lemma 4.7. We derive a parameterized matrix equation equivalent to $N(P) = P - (F'_{V\tilde{D}^{(j)}})^{-1}(F(P))$ and show that $\langle V\tilde{D}^{(j)}, P_\varepsilon\rangle$ includes the solution set of the matrix equation, i.e., we proceed with the proof similarly to section 3.3.

Since $\|t\|_\infty < 1$ and $\|\tau\|_\infty < 1$, Z_Q, T, and P are nonsingular. We obtain $N(P) = P - (F'_{V\tilde{D}^{(j)}})^{-1}(F(P)) \Leftrightarrow F'_{V\tilde{D}^{(j)}}(N(P)) = F'_{V\tilde{D}^{(j)}}(P) - F(P)$ and

$$\begin{aligned} F'_{V\tilde{D}^{(j)}}(N(P)) &= ((\tilde{D}+Q)UU^T - VV^T)N(P) - UU^T N(P)\tilde{D}^{(j)},\\ F'_{V\tilde{D}^{(j)}}(P) - F(P) &= -UU^T P(\tilde{D}^{(j)} - V^T P) - (\tilde{D}+Q)V. \end{aligned}$$

Hence the parameterized matrix equation is

$$((\tilde{D}+Q)UU^T - VV^T)N_P - UU^T N_P \tilde{D}^{(j)} = -UU^T P(\tilde{D}^{(j)} - V^T P) - (\tilde{D}+Q)V, \tag{4.3}$$

where $N_P \in \mathbb{C}^{n\times n_j}$ is unknown and $P \in \langle V\tilde{D}^{(j)}, P_r\rangle$ is the parameter. We thus prove $|V\tilde{D}^{(j)} - N_P| \le P_\varepsilon$ for any P. Any P can be represented as $P = V\tilde{D}^{(j)} + \underline{P}_r$, where $\underline{P}_r \in \mathbb{C}^{n\times n_j}$ satisfies $|\underline{P}_r| \le P_r$. It then holds for any P that

$$\begin{aligned} &-UU^T P(\tilde{D}^{(j)} - V^T P) - (\tilde{D}+Q)V\\ &\quad = -UU^T(V\tilde{D}^{(j)} + \underline{P}_r)(\tilde{D}^{(j)} - V^T(V\tilde{D}^{(j)} + \underline{P}_r)) - (\tilde{D}+Q)V\\ &\quad = UU^T \underline{P}_r V^T \underline{P}_r - (\tilde{D}+Q)V. \end{aligned}$$

Therefore (4.3) is equivalent to $((\tilde{D}+Q)UU^T - VV^T)N_P - UU^T N_P \tilde{D}^{(j)} = UU^T \underline{P}_r V^T \underline{P}_r - (\tilde{D}+Q)V$, where $\underline{P}_r \in \langle 0, P_r\rangle$, which can be written as $\mathsf{P}\mathrm{vec}(N_P) = \mathrm{vec}(UU^T \underline{P}_r V^T \underline{P}_r - (\tilde{D}+Q)V)$. Since P is nonsingular and $\tilde{D}V = V\tilde{D}^{(j)}$, it follows for any $\underline{P}_r$ that

$$\begin{aligned} \mathrm{vec}(V\tilde{D}^{(j)} - N_P) &= \mathrm{vec}(V\tilde{D}^{(j)}) - \mathrm{vec}(N_P)\\ &= \mathrm{vec}(V\tilde{D}^{(j)}) - \mathsf{P}^{-1}\mathrm{vec}(UU^T \underline{P}_r V^T \underline{P}_r - (\tilde{D}+Q)V)\\ &= \mathsf{P}^{-1}(\mathsf{P}\mathrm{vec}(V\tilde{D}^{(j)}) - \mathrm{vec}(UU^T \underline{P}_r V^T \underline{P}_r - (\tilde{D}+Q)V))\\ &= \mathsf{P}^{-1}\mathrm{vec}(QV - UU^T \underline{P}_r V^T \underline{P}_r). \end{aligned} \tag{4.4}$$

From (4.2) and the nonsingularity of Z_Q, on the other hand, we have

$$\begin{aligned} \mathsf{P} &= \begin{pmatrix} Z_Q & & \\ & \ddots & \\ & & Z_Q \end{pmatrix} \begin{pmatrix} I_n & & \\ \vdots & \ddots & \\ -\tilde{D}^{(j)}_{1n_j} Z_Q^{-1} UU^T & \cdots & I_n \end{pmatrix}\\ &= (I_{n_j} \otimes Z_Q)\left(\begin{pmatrix} I_n & & \\ & \ddots & \\ & & I_n \end{pmatrix} - \begin{pmatrix} 0 & & \\ \vdots & \ddots & \\ \tilde{D}^{(j)}_{1n_j} Z_Q^{-1} UU^T & \cdots & 0 \end{pmatrix}\right)\\ &= (I_{n_j} \otimes Z_Q)(I_{nn_j} - \Delta^T \otimes Z_Q^{-1} UU^T). \end{aligned} \tag{4.5}$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Since Δ is strictly upper triangular, $\Delta^p = (\Delta^T)^p = 0$ holds for integers p satisfying $p \geq n_j$. This, (4.5), $\rho(\Delta^T \otimes Z_Q^{-1}UU^T) = 0$, the Neumann series and Lemma 2.2 yield

$$\begin{aligned}
\mathsf{P}^{-1} &= (I_{nn_j} - \Delta^T \otimes Z_Q^{-1}UU^T)^{-1}(I_{n_j} \otimes Z_Q)^{-1} \\
&= (I_{nn_j} + \Delta^T \otimes Z_Q^{-1}UU^T + (\Delta^T \otimes Z_Q^{-1}UU^T)^2 + \cdots)(I_{n_j} \otimes Z_Q^{-1}) \\
&= (I_{nn_j} + \Delta^T \otimes Z_Q^{-1}UU^T + \Delta^{T^2} \otimes (Z_Q^{-1}UU^T)^2 + \cdots)(I_{n_j} \otimes Z_Q^{-1}) \\
&= (I_{nn_j} + \Delta^T \otimes Z_Q^{-1}UU^T + \cdots + \Delta^{T^{n_j-1}} \otimes (Z_Q^{-1}UU^T)^{n_j-1})(I_{n_j} \otimes Z_Q^{-1}) \\
&= I_{n_j} \otimes Z_Q^{-1} + \Delta^T \otimes Z_Q^{-1}UU^T Z_Q^{-1} + \cdots + \Delta^{T^{n_j-1}} \otimes (Z_Q^{-1}UU^T)^{n_j-1} Z_Q^{-1}.
\end{aligned}$$

This, (4.4), and Lemma 2.2 give

$$\begin{aligned}
\mathrm{vec}(V\tilde{D}^{(j)} - N_P) &= \left(\sum_{p=0}^{n_j-1} \Delta^{T^p} \otimes (Z_Q^{-1}UU^T)^p Z_Q^{-1} \right) \mathrm{vec}(QV + UU^T \underline{P}_r V^T \underline{P}_r) \\
&= \mathrm{vec} \left(\sum_{p=0}^{n_j-1} (Z_Q^{-1}UU^T)^p Z_Q^{-1}(QV + UU^T \underline{P}_r V^T \underline{P}_r)\Delta^p \right),
\end{aligned}$$

so that, abbreviating $Q_P := |Q|V + UU^T|\underline{P}_r|V^T|\underline{P}_r|$,

$$|V\tilde{D}^{(j)} - N_P| \leq \sum_{p=0}^{n_j-1} (|Z_Q^{-1}|UU^T)^p |Z_Q^{-1}| Q_P |\Delta|^p. \tag{4.6}$$

Similarly to the proof of Lemma 3.10, we have $|Q|V \leq R_w$, so that $Q_P \leq R_P$. The inequality $\|\tau\|_\infty < 1$, Corollary 2.4, and $|I_n - TZ_Q|\mathbb{1} \leq \tau$ moreover yield

$$|Z_Q^{-1}| = |Z_Q^{-1}T^{-1}T| = |(I_n - (I_n - TZ_Q))^{-1}T| \leq |(I_n - (I_n - TZ_Q))^{-1}||T| \leq \overline{T}.$$

This, $Q_P \leq R_P$, and (4.6) show $|V\tilde{D}^{(j)} - N_P| \leq P_\varepsilon$ for any $\underline{P}_r$, i.e., for any P. ∎

Remark 4.9. Let $\hat{\mathsf{P}} := \mathsf{P} - I_{n_j} \otimes QUU^T$. Lemmas 4.7 and 4.8 enable us to avoid computing $\mathrm{fl}(\hat{\mathsf{P}}^{-1})$ explicitly, which requires $\mathcal{O}(n^2 n_j^3 + n n_j^2 \sum_{p=1, j_p \neq j}^{m-k} n_{j_p}^2)$ operations.

THEOREM 4.10. *Let $\tilde{X}$, U, V, $\tilde{\lambda}$, and P_r be as above, Δ and P_ε be as in Lemma* 4.8, *and $\overline{P}_\varepsilon \geq P_\varepsilon$. If all the assumptions in Lemma* 4.7 *are true and $\overline{P}_\varepsilon < P_r$, then n_j eigenvalues of* (1.1) *is included in $\langle \tilde{\lambda}, \overline{\rho}(|\Delta| + V^T\overline{P}_\varepsilon) \rangle$ and $\langle \tilde{X}V, |\tilde{X}|UU^T\overline{P}_\varepsilon \rangle$ includes a matrix spanning the corresponding invariant subspace.*

Proof. Let Λ be as above. The result follows from a discussion similar to the proof of Theorem 3.11 and $\Lambda = V^T P \in V^T \langle V\tilde{D}^{(j)}, \overline{P}_\varepsilon \rangle \subseteq \langle \tilde{D}^{(j)}, V^T\overline{P}_\varepsilon \rangle = \langle \tilde{\lambda} I_{n_j} + \Delta, V^T\overline{P}_\varepsilon \rangle \subseteq \langle \tilde{\lambda} I_{n_j}, |\Delta| + V^T\overline{P}_\varepsilon \rangle$. ∎

COROLLARY 4.11. *Let P_r be as above, R_w and P_ε be as in Lemma* 4.8, *$\underline{P}_\varepsilon^*$ be P_ε when $P_r = 0$, $\sigma, \eta \in \mathbb{F}$, $\underline{P}_\varepsilon \in \mathbb{F}^{n \times n_j}$, and $\overline{P}_\varepsilon := \mathrm{fl}_\triangle((1 + \sigma\eta^2)\underline{P}_\varepsilon)$. Assume $\mathrm{fl}_\triangle(\cdot)$, $\underline{P}_\varepsilon$, R_w, σ, $\sigma(1 + \mathtt{eps})^6$, η, and P_r satisfy the conditions in Theorem* 3.15. *Then $P_\varepsilon \leq \overline{P}_\varepsilon < P_r$ follows.*

Proof. The analogy of the proof of Theorem 3.15 shows the result. ∎

4.3. Proposed algorithm. Based on the theories in sections 4.1 and 4.2, we propose an algorithm for enclosing all the eigenvalues and invariant subspaces.

ALGORITHM 3. *Let $\tilde{D}$, $\tilde{X}$, m, $\tilde{D}^{(1)}, \ldots, \tilde{D}^{(m)}$, $n_1, \ldots, n_m$, $j_1, \ldots, j_{m-k}$, R, and t be as in this section. This algorithm encloses all the eigenvalues and invariant subspaces based on the theories in sections* 4.1 *and* 4.2.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Step 1. *Compute* $\tilde{D}$ *and* $\tilde{X}$ *by the numerical BD.*

Step 2. *For* $p = 1, \ldots, m-k$, *let* $\tilde{\lambda}_{j_p} = \mathrm{fl}((\sum_{q=1}^{n_{j_p}} \tilde{D}_{qq}^{(j_p)})/n_{j_p})$ *and update* $\tilde{D}^{(j_p)}$ *such that* $\tilde{D}_{qq}^{(j_p)} = \tilde{\lambda}_{j_p}$, $q = 1, \ldots, n_{j_p}$.

Step 3. *Compute* $Y = \mathrm{fl}((B\tilde{X})^{-1})$, $\overline{\mathrm{fl}}(|R|)$, *and* $\overline{\mathrm{fl}}(t)$. *If* $\overline{\mathrm{fl}}(\|t\|_\infty) \geq 1$, *terminate with failure.*

Step 4. *Execute the following procedure for* $p = 1, \ldots, m$: *If* $n_p = 1$, *let* $\tilde{\lambda} := \tilde{D}^{(p)}$ *and* $i := \sum_{q=1}^{p-1} n_q + 1$, *and enclose one eigenvalue and its corresponding eigenvector by Algorithm* 4. *Otherwise let* $j = p$ *and enclose* n_j *eigenvalues and corresponding invariant subspace by Algorithm* 5. *Terminate.*

ALGORITHM 4. *Let* $\tilde{\lambda}$, i, U, T, τ, w, $\overline{w}$, $\underline{\xi}^*$, $\underline{\xi}$, $\overline{\xi}$, σ, *and* η *be as in section* 4.1, *and assume* $\mathrm{fl}_\triangle(\cdot)$ *satisfies the condition in Theorem* 3.15. *This algorithm encloses one eigenvalue and its corresponding eigenvector based on the theories in section* 4.1.

Step 1. *Compute* $T = \mathrm{fl}(((\tilde{D} - \tilde{\lambda} I_n)UU^T - e^{(i)}e^{(i)^T})^{-1})$ *and* $\overline{\mathrm{fl}}(\tau)$. *If* $\overline{\mathrm{fl}}(\|\tau\|_\infty) \geq 1$, *terminate with failure.*

Step 2. *Compute* $\overline{w} = \overline{\mathrm{fl}}(w + \|w\|_t t)$. *If* $\overline{w}_p < \sqrt{\texttt{realmin}}$ *for* $p \in \{1, \ldots, n\}$, *update* $\overline{w}_p$ *such that* $\overline{w}_p = \sqrt{\texttt{realmin}}$ $\forall$ p *satisfying this inequality.*

Step 3. *Compute* $\underline{\xi} = \overline{\mathrm{fl}}(\underline{\xi}^*)$ *and* $\sigma = \overline{\mathrm{fl}}(\|(UU^T\underline{\xi}e^{(i)^T}\underline{\xi})./\overline{w}\|_\infty)$. *If* $\overline{\mathrm{fl}}(\sigma(1+\texttt{eps})^6) \geq 1/4$, *terminate with failure.*

Step 4. *Let* $\eta = \overline{\mathrm{fl}}(2(1+\texttt{eps})^3/(1+\sqrt{1-4\sigma(1+\texttt{eps})^6}))$. *If* $\eta < (1+\sqrt{1-4\sigma(1+\texttt{eps})^6})/(2\sigma(1+\texttt{eps})^4)$ *cannot be verified, terminate with failure.*

Step 5. *Compute* $\overline{\xi} = \mathrm{fl}_\triangle((1+\sigma\eta^2)\underline{\xi})$ *and* $\overline{\mathrm{fl}}(|\tilde{X}|UU^T\overline{\xi})$. *Terminate.*

ALGORITHM 5. *Let* j, U, V, Z, T, τ, w, R_w, Δ, $\underline{P}_\varepsilon^*$, $\underline{P}_\varepsilon$, $\overline{P}_\varepsilon$, σ, *and* η *be as in section* 4.2, *and assume* $\mathrm{fl}_\triangle(\cdot)$ *satisfies the condition. This algorithm encloses* n_j *eigenvalues and corresponding invariant subspace based on the theories in section* 4.2.

Step 1. *Compute* $T = \mathrm{fl}(Z^{-1})$ *and* $\overline{\mathrm{fl}}(\tau)$. *If* $\overline{\mathrm{fl}}(\|\tau\|_\infty) \geq 1$, *terminate with failure.*

Step 2. *Compute* $\hat{R} := \overline{\mathrm{fl}}(|R|V + tw^T)$. *If* $\hat{R}_{pq} < \sqrt{\texttt{realmin}}$ *for* $p \in \{1, \ldots, n\}$ *and* $q \in \{1, \ldots, n_j\}$, *update* $\hat{R}_{pq}$ *such that* $\hat{R}_{pq} = \sqrt{\texttt{realmin}}$ $\forall$ *pairs of* p *and* q *satisfying this inequality. Compute* $r^w \in \mathbb{R}^n$ *and* R_w *such that* $r_p^w := \max_q \hat{R}_{pq}$, $p = 1, \ldots, n$, *and* $R_w = r^w \mathbb{1}^T$, *respectively.*

Step 3. *Compute* $\underline{P}_\varepsilon = \overline{\mathrm{fl}}(\underline{P}_\varepsilon^*)$ *and* $\sigma = \overline{\mathrm{fl}}(\|(UU^T\underline{P}_\varepsilon V^T \underline{P}_\varepsilon)./R_w\|_{\mathrm{M}})$. *If* $\overline{\mathrm{fl}}(\sigma(1+\texttt{eps})^6) \geq 1/4$, *terminate with failure.*

Step 4. *Let* $\eta = \overline{\mathrm{fl}}(2(1+\texttt{eps})^3/(1+\sqrt{1-4\sigma(1+\texttt{eps})^6}))$. *If* $\eta < (1+\sqrt{1-4\sigma(1+\texttt{eps})^6})/(2\sigma(1+\texttt{eps})^4)$ *cannot be verified, terminate with failure.*

Step 5. *Compute* $\overline{P}_\varepsilon = \mathrm{fl}_\triangle((1+\sigma\eta^2)\underline{P}_\varepsilon)$, $\overline{\mathrm{fl}}(|\tilde{X}|UU^T\overline{P}_\varepsilon)$, *and* $\overline{\rho}(|\Delta| + V^T\overline{P}_\varepsilon)$. *Terminate.*

Remark 4.12. If Algorithm 3 terminated without failure and all the obtained disks enclosing eigenvalues are isolated mutually, then these disks do not contain common eigenvalues, i.e., the union of these disks includes all the eigenvalues.

Algorithm 4 contains the computation of T and matrix multiplication $T((\tilde{D} - \tilde{\lambda} I_n)UU^T - e^{(i)}e^{(i)^T})$, which require $\mathcal{O}(\sum_{p=1}^{m-k} n_{j_p}^3)$ operations. The computational cost of the other part in Algorithm 4 is $\mathcal{O}(n^2)$. Hence the computational cost of Algorithm 4 is $\mathcal{O}(\sum_{p=1}^{m-k} n_{j_p}^3 + n^2)$.

The computation of T and the matrix multiplication TZ in Algorithm 5 require $\sum_{p=1, j_p \neq j}^{m-k} n_{j_p}^3$ operations. Since R_w in Algorithm 5 is constructed as $R_w = r^w \mathbb{1}^T$, we have $\underline{P}_\varepsilon^* = \sum_{p=0}^{n_j - 1} (\overline{T}UU^T)^p \overline{T} r^w \mathbb{1}^T |\Delta|^p$. The matrix-vector multiplications $(\overline{T}UU^T)^p \overline{T} r^w$, $p = 0, \ldots, n_j - 1$, involve $\mathcal{O}(n^2 n_j)$ operations in total. The vector-matrix multiplications $\mathbb{1}^T |\Delta|^p$, $p = 1, \ldots, n_j - 1$, require $\mathcal{O}(n_j^3)$ operations in total.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

The outer products $((\overline{T}UU^T)^p\overline{T}r^w)(\mathbb{1}^T|\Delta|^p)$, $p = 0, \ldots, n_j - 1$, involve $\mathcal{O}(nn_j^2)$ operations in total. The sum within $\underline{P}_\varepsilon^*$ requires $\mathcal{O}(nn_j^2)$ operations. The matrix multiplications $UU^T\underline{P}_\varepsilon V^T\underline{P}_\varepsilon$ and $|\tilde{X}|UU^T\overline{P}_\varepsilon$ involve $\mathcal{O}(nn_j^2)$ and $\mathcal{O}(n^2n_j)$ operations, respectively. The computation of $\overline{\rho}(|\Delta| + V^T\overline{P}_\varepsilon)$ involves at most $\mathcal{O}(n_j^3)$ operations. The computational cost of the other parts are $\mathcal{O}(n^2)$. From the above, the computational cost of Algorithm 5 is $\mathcal{O}(n^2n_j + nn_j^2 + \sum_{p=1}^{m-k} n_{j_p}^3)$.

In Algorithm 3, the computations of $\tilde{D}$, $\tilde{X}$, Y, $\overline{\mathrm{fl}}(|R|)$, and $\overline{\mathrm{fl}}(t)$ require $\mathcal{O}(n^3)$ operations. Algorithms 4 and 5 are executed k and $m-k$ times, and the k and $m-k$ times executions involve $\mathcal{O}(k\sum_{p=1}^{m-k} n_{j_p}^3 + kn^2)$ and $\mathcal{O}(n^2\sum_{p=1}^{m-k} n_{j_p} + n\sum_{p=1}^{m-k} n_{j_p}^2 + (m-k)\sum_{p=1}^{m-k} n_{j_p}^3)$ operations, respectively. From this and $k + \sum_{p=1}^{m-k} n_{j_p} = n$, the computational cost of Algorithm 3 is $\mathcal{O}(n^3 + n\sum_{p=1}^{m-k} n_{j_p}^2 + m\sum_{p=1}^{m-k} n_{j_p}^3)$. We obtain

$$\begin{aligned} n^3 + n\sum_{p=1}^{m-k} n_{j_p}^2 + m\sum_{p=1}^{m-k} n_{j_p}^3 &< n^3 + n\left(\sum_{p=1}^{m-k} n_{j_p}\right)^2 + m\left(\sum_{p=1}^{m-k} n_{j_p}\right)^3 \\ &\le n^3 + nn^2 + mn^3 = (m+2)n^3, \end{aligned}$$

which implies that the cost of Algorithm 3 is smaller than $\mathcal{O}(mn^3)$. When we enclose all the eigenvalues and invariant subspaces by the known algorithms, alternatively, $\mathcal{O}(mn^3)$ operations are required except the case when A and B have special structures (e.g., A is Hermitian and B is Hermitian positive definite). For instance, when we enclose the eigenvalues and individual eigenvectors, and the eigenvalues and invariant subspaces regarding to $\tilde{D}^{(i_1)}, \ldots, \tilde{D}^{(i_k)}$ and $\tilde{D}^{(j_1)}, \ldots, \tilde{D}^{(j_{m-k})}$ by repeatedly executing the algorithms in [8] and [9], $\mathcal{O}(kn^3)$ and $\mathcal{O}((m-k)n^3)$ operations are required in total, respectively.

5. Numerical results. In this section, we report numerical results to observe the properties of Algorithms 1 and 3 and performance of our implementation. We used a computer with an Intel Xeon 2.66-GHz Dual CPU, 4.00 GB RAM, and MATLAB 7.5 with the Intel Math Kernel Library and IEEE 754 double precision. In this environment, $\mathrm{fl}_\triangle(\cdot)$ satisfies the condition in Theorem 3.15 except the cases of underflow and overflow.

In most of the compared algorithms, eigenvalue clusters have to be determined manually. In fact, the BD requires the manual determination. We thus introduce a positive real number `tol`. Let $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$ be approximate eigenvalues, $i, j \in \{1, \ldots, n\}$, and $i \neq j$. In these algorithms, if $\mathrm{fl}(|\tilde{\lambda}_i - \tilde{\lambda}_j|) \le$ `tol`, $\tilde{\lambda}_i$ and $\tilde{\lambda}_j$ are allocated to the same eigenvalue cluster. Otherwise they are allocated to the different clusters.

We denote the compared algorithms as follows:

M1: Algorithm 1, where the eigenvalue clusters are automatically determined.
M2a: Algorithm 3 with `tol` = 1e–8.
M2b: Algorithm 3 with `tol` = 1e–6.
V1a: An algorithm for enclosing all the eigenvalues and invariant subspaces by executing the GED and repeatedly calling the INTLAB [17] function `verifyeig` with `tol` = 1e–8.
V1b: An analogous of V1a with `tol` = 1e–6.
V2a: An analogous of V1a executing the BD with `tol` = 1e–8 instead of the GED.
V2b: An analogous of V2a with `tol` = 1e–6.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

TABLE 1

Maximum radii for eigenvalues (upper part), invariant subspaces (middle part), and computing times (lower part) in Example 5.1.

n	M1	M2a	M2b	V1a	V1b	V2a	V2b
100	4.5e–10	4.4e–11	4.4e–11	4.5e–11	4.5e–11	4.5e–11	4.5e–11
300	1.5e–8	6.8e–10	6.8e–10	8.9e–10	8.9e–10	8.9e–10	8.9e–10
500	2.4e–8	5.5e–10	5.5e–10	8.1e–10	8.1e–10	8.0e–10	8.0e–10
700	3.0e–8	3.1e–10	3.1e–10	5.1e–10	5.1e–10	5.1e–10	5.1e–10
100	1.2e–11	1.5e–11	1.5e–11	9.0e–13	9.0e–13	1.5e–12	1.5e–12
300	1.6e–10	3.0e–10	3.0e–10	1.5e–11	1.5e–11	3.6e–11	3.6e–11
500	7.3e–10	4.0e–9	4.0e–9	7.7e–11	7.7e–11	4.3e–10	4.3e–10
700	1.1e–9	4.2e–9	4.2e–9	1.1e–10	1.1e–10	4.0e–10	4.0e–10
100	0.200	0.488	0.487	2.967	2.963	2.985	2.991
300	4.643	11.67	11.67	125.0	124.9	125.6	125.6
500	20.61	56.34	56.25	714.9	712.6	721.1	721.2
700	57.91	157.4	157.8	2328	2335	2352	2349

In M1, V1a, and V1b, the GED was executed by the MATLAB function `eig`. In the computation of $\overline{\rho}(V^T\overline{P}_\varepsilon)$ and $\overline{\rho}(|\Delta| + V^T\overline{P}_\varepsilon)$ based on [9, section 3], approximate Perron vectors of these matrices are required. In M1, M2a, and M2b, the Perron vectors were obtained by `eig`, and Y was computed by the MATLAB command `\`. Note that `verifyeig` also obtains the Perron vectors by `eig`. Let $\tilde{\lambda}_{i_1}, \ldots, \tilde{\lambda}_{i_k}$ be all the approximate eigenvalues belong to the same eigenvalue cluster. In V1a, V1b, V2a, and V2b, $\mathrm{fl}((\sum_{p=1}^{k} \tilde{\lambda}_{i_p})/k)$ was input to `verifyeig` as an approximate eigenvalue. The function `bdschur` in MATLAB Control System Toolbox executes the BD in [12], so this function is not suited for our purpose (see Remark 4.1). We thus executed the BD by the code in the appendix.

Let $d^r \in \mathbb{R}^n$ and $X^r \in \mathbb{R}^{n\times n}$ have nonnegative components, and $\langle \tilde{\lambda}_i, d_i^r\rangle$, $i = 1, \ldots, n$, and $\langle \tilde{X}, X^r\rangle$ enclose all the eigenvalues and invariant subspaces, respectively. In order to assess the qualities of the enclosures, we define the maximum radii for eigenvalues and invariant subspaces as $\max_i d_i^r$ and $\max_{i,j} X_{ij}^r$, respectively. In the examples below, the compared algorithms failed in the enclosure of some eigenvalues and corresponding invariant subspaces. We thus display the number of eigenvalues for which the algorithms failed. In this case, the maximum radii are the maximum value obtained from the radii of the succeeded results. In M1, M2a, and M2b, when the number of failures was zero, it was guaranteed that they enclosed *all* the eigenvalues (see Remarks 3.18 and 4.12). For nonsingular $M \in \mathbb{C}^{n\times n}$, define the condition number $\kappa(M) := \|M\|_2\|M^{-1}\|_2$. M1, M2a, and M2b verified the nonsingularity of B for examples in which the numbers of failures were smaller than n. In Tables 2 and 3, the notations fail_t, fail_Y, and $\mathrm{fail}_{\tau\sigma}$ mean that M1, M2a, or M2b failed since $\|t\|_\infty < 1$ could not be verified, `NaN` is included in Y, and $\|\tau\|_\infty < 1$ or $\sigma(1+\mathtt{eps})^6 < 1/4$ could not be verified for all the blocks, respectively. The notation $\mathrm{fail}_{\mathtt{V}}$ means that V1a, V1b, V2a, or V2b returned `NaN` for all the clusters.

Example 5.1. In this example, we observe the magnitudes of the radii and computing times for various n. Consider the case when $n\times n$ complex matrices A and B are generated by the following MATLAB code

```
A = randn(n) + i*randn(n);  B = randn(n) + i*randn(n);
```

Then the real and imaginary parts of the entries in A and B are pseudorandom numbers uniformly distributed in $[-1, 1]$. Table 1 displays the maximum radii and

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

TABLE 2
Maximum radii for eigenvalues (upper part), invariant subspaces (middle part), and numbers of failure (lower part) in Example 5.2.

`cnd`	M1	M2a	M2b	V1a	V1b	V2a	V2b
1e+4	4.2e–9	1.1e–10	1.1e–10	1.0e–10	1.0e–10	1.0e–10	1.0e–10
1e+8	4.8e–6	4.0e–7	4.0e–7	3.7e–10	3.7e–10	3.7e–10	3.7e–10
1e+12	1.8e–2	2.3e–3	2.8e–3	5.7e–14	5.7e–14	5.7e–14	5.7e–14
1e+13	fail_t	4.9e–2	$\mathrm{fail}_{\tau\sigma}$	1.2e–15	$\mathrm{fail}_{\mathtt{V}}$	1.2e–15	$\mathrm{fail}_{\mathtt{V}}$
1e+4	5.9e–10	1.3e–9	1.3e–9	1.1e–10	1.1e–10	3.1e–10	3.1e–10
1e+8	1.1e–6	1.9e–6	1.9e–6	2.6e–8	2.6e–8	3.3e–8	3.3e–8
1e+12	6.8e–3	9.4e–3	1.2e–2	1.6e–8	1.6e–8	2.7e–8	2.0e–8
1e+13	fail_t	2.4e–1	$\mathrm{fail}_{\tau\sigma}$	6.7e–9	$\mathrm{fail}_{\mathtt{V}}$	8.4e–9	$\mathrm{fail}_{\mathtt{V}}$
1e+4	0	0	0	0	0	0	0
1e+8	0	0	13	27	40	27	40
1e+12	0	27	43	80	96	80	96
1e+13	100	78	100	89	100	89	100

computing times (sec) of the algorithms. In this example, all the algorithms succeeded for all the eigenvalues.

It can be seen from Table 1 that the radii obtained by the algorithms were comparable. The algorithms M1, M2a, and M2b were much faster than V1a, V1b, V2a, and V2b. The reason is as follows: In these examples, all the eigenvalues were well separated. Hence `verifyeig` was called n times in the latter algorithms, so that they required $\mathcal{O}(n^4)$ operations. On the other hand, the former algorithms required only $\mathcal{O}(n^3)$ operations.

Example 5.2. In this example, we observe the properties of the algorithms when $\kappa(B)$ increases. We generated 100×100 complex matrices A and B by the code

```
A = randn(100) + i*randn(100);
cnd10 = log10(cnd);  % cnd: anticipated condition number of B
D = diag(logspace(0,cnd10,100));
[U,S,V] = svd(randn(100) + i*randn(100));  B = U*D*V';
```

Then it holds approximately that $\kappa(B) \approx$ `cnd`. Table 2 displays the maximum radii and numbers of eigenvalues for which the algorithms failed for various `cnd`.

From Table 2, when `cnd` = 1e+8, 1e+12, the radii by V1a, V1b, V2a, and V2b seem to be smaller than those by M1, M2a, and M2b. However, this comparison is not fair. The reason is that the numbers of the failure in the former algorithms are larger than those in the latter algorithms. The number of the failure in M2b was larger than those in M2a. The reason is guessed as follows: The sum $\sum_{p=1}^{m-k} n_{j_p}$ in M2b was larger than that in M2a, so that the number of the updated diagonal element of $\tilde{D}$ in M2b was also larger than that in M2a. This caused loss of accuracy of $\tilde{D}$, i.e., enlargement of several components of $|R|$. From this enlargement, the conditions in Algorithms 4 or 5 could not be verified.

Example 5.3. In this example, we observe the properties of the algorithms in the case when (1.1) has defective eigenvalues. Let

$$A_0 := \begin{pmatrix} 2 & 2 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \text{ whose Jordan canonical form is } \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

TABLE 3
Maximum radii for eigenvalues (upper part), invariant subspaces (middle part), and numbers of failure (lower part) in Example 5.3.

m	M1	M2a	M2b	V1a	V1b	V2a	V2b
4	fail$_Y$	fail$_Y$	3.2e–2	fail$_V$	fail$_V$	fail$_V$	4.9e–4
5	fail$_Y$	fail$_t$	4.5e–2	fail$_V$	fail$_V$	fail$_V$	5.6e–4
6	fail$_Y$	fail$_Y$	3.3e–2	fail$_V$	fail$_V$	fail$_V$	1.9e–3
7	fail$_Y$	fail$_t$	fail$_t$	fail$_V$	fail$_V$	fail$_V$	fail$_V$
4	fail$_Y$	fail$_Y$	8.3e–3	fail$_V$	fail$_V$	fail$_V$	4.6e–5
5	fail$_Y$	fail$_t$	2.8e–2	fail$_V$	fail$_V$	fail$_V$	1.9e–4
6	fail$_Y$	fail$_Y$	5.0e+1	fail$_V$	fail$_V$	fail$_V$	8.4e–3
7	fail$_Y$	fail$_t$	fail$_t$	fail$_V$	fail$_V$	fail$_V$	fail$_V$
4	16	16	0	16	16	16	4
5	20	20	0	20	20	20	4
6	24	24	0	24	24	24	8
7	28	28	28	28	28	28	28

Hence 1 is the four-fold defective eigenvalue of A_0. Let also $B = I_n$ and

$$A = \begin{pmatrix} A_0 & A^{(1,2)} & & \cdots & A^{(1,m)} \\ & 2A_0 & A^{(2,3)} & \cdots & A^{(2,m)} \\ & & \ddots & \ddots & \vdots \\ & & & (m-1)A_0 & A^{(m-1,m)} \\ & & & & mA_0 \end{pmatrix},$$

where $A^{(1,2)}, \ldots, A^{(m-1,m)}$ are random submatrices generated by `randn`. Then A is block upper triangular having m Jordan block of size 4, so that (1.1) has four-fold defective eigenvalues $1, \ldots, m$. Table 3 displays quantities similar to Table 2 for various m. Note that $A_0, \ldots, mA_0$ can be stored exactly in the double precision floating point numbers for m in these tables.

M1 and M2a failed for all the problems. M2b succeeded when $m = 4, 5, 6$, however, even if (1.1) has defective eigenvalues. The reason M2a and M2b failed and succeeded, respectively, is as follows: Let $\tilde{\lambda}_p$ and $\tilde{\lambda}_q$ be the approximations of the same defective eigenvalue. Then $1\text{e–}8 < \mathrm{fl}(|\tilde{\lambda}_p - \tilde{\lambda}_q|) \leq 1\text{e–}6$ followed for most of the approximations. In M2a, therefore, these approximations were allocated to different blocks, so that $\kappa(\tilde{X})$ was extremely large, and fail$_t$ or fail$_Y$ occurred. In M2b, however, these approximations were allocated to the same block, so that $\kappa(\tilde{X})$ was not too large. When $m = 7$, alternatively, M2b failed since $\kappa(\tilde{X})$ was too large. In fact, $\kappa(\tilde{X})$ in M2b increased as m increased, although four approximations of the each defective eigenvalue were allocated to the same block in all the cases. Clarifying the reason for the increase of $\kappa(\tilde{X})$ will be our future work.

6. Appendix.

In what follows we display the MATLAB code for executing the BD discussed in this paper, where `lyap` is the function in the Control System Toolbox which solves the Sylvester equation.

```
function [X,D,Blks] = bdg(A,B,tol)
% BDG executes the BD, where Blks is the vector of block sizes.
% tol is a tolerance for determining eigenvalue clusters, i.e. blocks.

[X,D] = schur(B\A,'complex');  % Schur decomposition

% computation of cluster index vector
```

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

```
flg = ones(n,1);  % flag showing approximate eigenvalues are not allocated
cv_ctr = 1;       % cluster index counter
cv = zeros(n,1);  % cluster index vector
d = diag(D);  idx = 1;  clt = 1;  flg(1) = 0;  val = d(1);  d(1) = inf;
while max(flg) == 1
  [min_dst,min_idx] = min(abs(val - d));
  if min_dst > tol  % the cluster is separated from the other
    cv(clt) = cv_ctr;  cv_ctr = cv_ctr + 1;
    idx = find(flg,1,'first');  clt = idx;
    flg(idx) = 0;  val = d(idx);  d(idx) = inf;
  else
    clt = [clt;min_idx];  d(min_idx) = inf;  flg(min_idx) = 0;
  end
end
cv(clt) = cv_ctr;

[X,D] = ordschur(X,D,cv);  % Schur decomposition with reordering

% elimination of off-diagonal elements
idx = 1;  Blks = [];  ctr = 0;  % ctr: block size counter
while idx + ctr <= n-1
  if abs(D(idx,idx) - D(idx+ctr+1,idx+ctr+1)) > tol  % elimination possible
    V = lyap(D(idx:idx+ctr,idx:idx+ctr),-D(idx+ctr+1:end,idx+ctr+1:end),...
             D(idx:idx+ctr,idx+ctr+1:end));  % solving Sylvester equation
    D(idx:idx+ctr,idx+ctr+1:end) = 0;        % elimination
    X(:,idx+ctr+1:end) = X(:,idx:idx+ctr)*V + X(:,idx+ctr+1:end);
    idx = idx + ctr + 1;  Blks = [Blks;ctr+1];  ctr = 0;
  else
    ctr = ctr + 1;
  end
end
Blks = [Blks;ctr+1];
```

Acknowledgment. The author acknowledges Prof. Siegfried M. Rump of Hamburg University of Technology and Mr. Atsushi Minamihata of Waseda University for fruitful discussions. The author also thanks the referees for valuable comments.

REFERENCES

[1] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd ed., Johns Hopkins University Press, Baltimore, 1996.

[2] H. Behnke, *Inclusion of eigenvalues of general eigenvalue problems for matrices*, Computing Suppl., 6 (1988), pp. 69–78.

[3] H. Behnke, *The calculation of guaranteed bounds for eigenvalues using complementary variational principles*, Computing, 47 (1991), pp. 11–27.

[4] K. Maruyama, T. Ogita, Y. Nakaya, and S. Oishi, *Numerical inclusion method for all eigenvalues of real symmetric definite generalized eigenvalue problem* (in Japanese), IEICE Trans., J87-A (2004), pp. 1111–1119.

[5] S. Miyajima, *Fast enclosure for all eigenvalues in generalized eigenvalue problems*, J. Comput. Appl. Math., 233 (2010), pp. 2994–3004.

[6] S. Miyajima, *Numerical enclosure for each eigenvalue in generalized eigenvalue problem*, J. Comput. Appl. Math., 236 (2012), pp. 2545–2552.

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.

[7] S. Miyajima, T. Ogita, S. M. Rump, and S. Oishi, *Fast verification for all eigenpairs in symmetric positive definite generalized eigenvalue problems*, Reliab. Comput., 14 (2010), pp. 24–45.

[8] S. M. Rump, *Guaranteed inclusions for the complex generalized eigenproblem*, Computing, 42 (1989), pp. 225–238.

[9] S. M. Rump, *Computational error bounds for multiple or nearly multiple eigenvalues*, Linear Algebra Appl., 324 (2001), pp. 209–226.

[10] Y. Watanabe, N. Yamamoto, and M. T. Nakao, *Verification methods of generalized eigenvalue problems and its applications* (in Japanese), Trans. JSIAM, 9 (1999), pp. 137–150.

[11] N. Yamamoto, *A simple method for error bounds of eigenvalues of symmetric matrices*, Linear Algebra Appl., 324 (2001), pp. 227–234.

[12] A. Bavely and G. Stewart, *An algorithm for computing reducing subspaces by block diagonalization*, SIAM J. Numer. Anal., 16 (1979), pp. 359–367.

[13] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis*, Cambridge University Press, Cambridge, UK, 1994.

[14] A. Minamihata, *private communication*, 2013.

[15] S. M. Rump and J. Zemke, *On eigenvector bounds*, BIT, 43 (2004), pp. 823–837.

[16] H. Arndt, *On the interval systems* $[x] = [A][x] + [b]$ *and the powers of interval matrices in complex interval arithmetics*, Reliab. Comput., 13 (2007), pp. 245–259.

[17] S. M. Rump, *INTLAB — INTerval LABoratory*, in Developments in Reliable Computing, T. Csendes, ed., Kluwer Academic Publishers, Dordrecht, Netherlands, 1999, pp. 77–107.

Downloaded 11/19/14 to 129.49.23.145. Redistribution subject to SIAM license or copyright; see http://www.siam.org/journals/ojsa.php

Copyright © by SIAM. Unauthorized reproduction of this article is prohibited.