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ON EIGENVECTOR BOUNDS

SIEGFRIED M. RUMP AND JENS-PETER M. ZEMKE *

Abstract. There are methods to compute error bounds for a multiple eigenvalue together with an inclusion of a basis of the corresponding invariant subspace. Those methods have no restriction with respect to the structure of Jordan blocks, but they do not provide an inclusion of a *single* eigenvector. In this note we first show under general assumptions that a narrow inclusion of a single eigenvector is not likely in case of corresponding eigenvalue with geometric multiplicity greater than one. We show a similar result if attention is restricted to symmetric or Hermitian matrices. Finally, we present an inclusion theorem for the eigenvector to an eigenvalue of geometric multiplicity one. Some numerical examples demonstrate the numerical applicability.

1. Introduction. Denote $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and let $A \in M_n(\mathbb{K})$. Denote the spectrum of A by $\mathrm{spec}(A)$ and let $\lambda \in \mathrm{spec}(A)$ be an eigenvalue of A.

For λ being a simple and isolated eigenvalue there are various methods known to compute error bounds for λ and the corresponding eigenvector. For a comprehensive overview see [6]. For a double or nearly double eigenvalues there are also self-validating methods for computing error bounds for λ and for a basis of the corresponding invariant subspace [1]. Recently, a method for multiple or nearly multiple eigenvalues was presented in [10]. Both methods do not allow to compute bounds (except trivial ones) for a single eigenvector to a multiple eigenvalue λ, i.e. some (narrow) $X \subseteq \mathbb{K}^n$ with $\exists\, 0 \neq x \in X : \; Ax = \lambda x$.

In numerical analysis various results are known on the distance or separation of eigenvectors ([12]). So the question may arise: Is it possible to compute (narrow) error bounds for a single eigenvector to a multiple or nearly multiple eigenvalue λ? Exactly this question was posed to the first author [7] and lead to this note.

We want to illustrate the problem by a practical example. Consider

$$B := \begin{pmatrix} 2 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad H := \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

such that B is a matrix with three-fold eigenvalue 2 in two Jordan blocks of size 2 and 1. We apply a similarity transformation using the 4×4 Hadamard matrix H and obtain

$$A := HBH^{-1} = \frac{1}{2} \begin{pmatrix} 4 & 0 & 1 & -1 \\ 1 & 3 & 0 & 0 \\ 1 & -1 & 4 & 0 \\ 0 & 0 & 1 & 3 \end{pmatrix}.$$

The matrices A and B have identical eigenvalues and Jordan structure. Eigenvectors of A to the eigenvalue 2 are the corresponding columns of H, that is $x_1 = (1\ 1\ 1\ 1)^T$ and $x_2 = (1\ 1\ -1\ -1)^T$, as well as linear combinations of those. Using the Matlab command $[V, D] = \mathrm{eig}(A)$ we obtain approximations to eigenvectors and eigenvalues of A. The three approximations of "eigenvectors" to the eigenvalue $\lambda = 2$ are

v_1	v_2	v_3
-4.999999839640428e-001	5.000000160359587e-001	-1.075269548441611e-001
-5.000000138021311e-001	4.999999861978696e-001	-1.075269548441583e-001
-4.999999861978680e-001	5.000000138021297e-001	-6.988833622157158e-001
-5.000000160359571e-001	4.999999839640413e-001	-6.988833622157139e-001

* Technical University Hamburg-Harburg, Schwarzenbergstr. 95, 21071 Hamburg, Germany

As to be expected by the Jordan structure of A two of the approximations, namely v_1 and v_2, are almost identical. We feed these approximations v into the inclusion algorithm for multiple eigenvalues described in [10] and as implemented in [9]. The resulting inclusion of the eigenvalue is included in

$$L := \{z \in \mathbf{C} : \ |z - 2.00000000062| \leq 3.1 \cdot 10^{-8}\},$$

and corresponding inclusions of a basis for the invariant subspace are included in

X_1	X_2	X_3
$-0.4999999839640428 \pm 1.2 \cdot 10^{-16}$	$0.5000000160359587 \pm 1.2 \cdot 10^{-16}$	$-0.1075269548441611 \pm 1.4 \cdot 10^{-17}$
$-0.5000000138021319 \pm 3.4 \cdot 10^{-16}$	$0.4999999861978704 \pm 1.7 \cdot 10^{-16}$	$-0.1075269548441592 \pm 8.4 \cdot 10^{-17}$
$-0.4999999861978680 \pm 5.6 \cdot 10^{-17}$	$0.5000000138021297 \pm 1.2 \cdot 10^{-16}$	$-0.6988833622157158 \pm 2.3 \cdot 10^{-16}$
$-0.5000000160359571 \pm 1.2 \cdot 10^{-16}$	$0.4999999839640413 \pm 1.2 \cdot 10^{-16}$	$-0.6988833622157139 \pm 1.2 \cdot 10^{-16}$

By nature of the problem, the inclusion L is complex, see [10]. The accuracy of L corresponds to the sensitivity $\varepsilon^{1/2} \approx 1.4 \cdot 10^{-8}$ of the eigenvalue $\lambda = 2$. Note that the X_ν, $1 \leq \nu \leq 3$, are an inclusion of a basis of the invariant subspace to the eigenvalue of A included in L, i.e. to $\lambda = 2$. The X_ν are *not* necessarily inclusions of eigenvectors. And indeed, any linear combination of the true eigenvectors x_1 and x_2 has identical first and second component, so neither X_1 nor X_2 nor X_3 contain an eigenvector of A. But every eigenvector to $\lambda = 2$ is a suitable linear combination of the X_ν.

If better approximations than v_1, v_2, v_3 are used, better inclusions are obtained. For example, using the exact values $\lambda = 2$ and the first three columns H_ν, $1 \leq \nu \leq 3$, of H produces the inclusion

$$L' := \{z \in \mathbf{C} : \ |z - 2| \leq 1.1 \cdot 10^{-15}\}$$

for the eigenvalue and

X'_1	X'_2	X'_3
$1 \pm 5.6 \cdot 10^{-16}$	$1 \pm 5.6 \cdot 10^{-16}$	$1 \pm 5.6 \cdot 10^{-16}$
1	-1	1
1	1	-1
1	-1	-1

for the basis of the corresponding invariant subspace. In this case only the first components of X'_ν are thick due to the integer entries of the problem. So sharp k-dimensional information about eigenvectors can be achieved, but not much more.

We will show that, unless the geometric multiplicity of λ is equal to one, it is indeed not likely that narrow bounds are possible at all. In a way this elaborates a statement by Wilkinson: "Of course it will be extremely difficult to prove *by computation involving rounding errors* that the original matrix has a non-linear divisor. However, it should be appreciated that it is virtually impossible to establish by such methods that a matrix has a multiple eigenvalue as long as rounding errors are made, [...]" [12, p. 187]. In order to *prove* a statement in that direction we need assumptions on the self-validating methods we have in mind.

Most if not all self-validating methods do verify the assumptions of an inclusion theorem with the aid of digital computers (cf. [11]). This verification process is performed in floating point arithmetic, mostly with directed roundings. Therefore it seems likely that the assumptions are not only satisfied for the original input data but also in some small epsilon-neighbourhood of the input data. We formalize this for our application by assuming a mathematical theorem to be given as follows.

ASSUMPTION 1.1. *Let* $\mathbb{K} \in \{\mathbb{R}, \mathbf{C}\}$, $A \in M_n(\mathbb{K})$, $\Lambda \subseteq \mathbb{K}$ *and* $X \subseteq \mathbb{K}^n$ *be given. If the predicate* $\Phi(A, \Lambda, X)$ *is satisfied, then there exists* $\widehat{\lambda} \in \Lambda$ *and* $0 \neq \widehat{x} \in X$ *with* $A\widehat{x} = \widehat{\lambda}\widehat{x}$.

In the light of our preceeding discussion the validity of the predicate $\Phi(A, \Lambda, X)$ is verified with the aid of a digital computer thereby proving validity of the assertions. But frequently $\Phi(\widetilde{A}, \Lambda, X)$ for $\widetilde{A} \in U_\varepsilon(A)$ is satisfied for small ε, proving validity of the assertions for $\widetilde{A}$ as well.

Our only hypotheses for this paper are i) that a predicate $\Phi : M_n(\mathbb{IK}) \times \mathbb{IPIK} \times \mathbb{IPIK}^n \to \{0,1\}$ is given such that the Assumption 1.1 is valid, and ii) that for given $A \in M_n(\mathbb{IK})$, $\Lambda \subseteq \mathbb{IK}$ and $X \subseteq \mathbb{IK}^n$ the predicate $\Phi(\widetilde{A}, \Lambda, X)$ is satisfied for all $\widetilde{A} \in U_\varepsilon(A)$. With this we will show that narrow inclusions X for a single eigenvector of an eigenvalue of geometric multiplicity greater than one is not likely. For the case of geometric multiplicity one – which is the generic case – we present an inclusion algorithm for the eigenvector.

In case of symmetric or, more general, in case of normal matrices the geometric and algebraic multiplicity of eigenvalues coincide. We show that even if we restrict the matrices in Assumption 1.1 to symmetric or Hermitian matrices, then still narrow inclusions for a single eigenvector are unlikely in case of a corresponding multiple or nearly multiple eigenvalue.

2. Geometric multiplicity greater equal 2. Suppose λ is of geometric multiplicity $g \geq 2$. Then there are g linearly independent eigenvectors of A to λ, spanning a g-dimensional subspace. This in turn is a subspace of the full invariant subspace to λ of dimension equal to the algebraic multiplicity of λ.

LEMMA 2.1. *For $A \in M_n(\mathbb{IK})$ let an eigenvalue $\lambda \in \mathrm{spec}(A)$ be given with algebraic multiplicity m, and let $0 \neq y \in \mathbb{IK}^n$ with $Ay = \lambda y$ be an eigenvector of A. Then for all $\varepsilon > 0$ there exists $\widetilde{A} \in U_\varepsilon(A)$ with the following properties:*

i) $\lambda \in \mathrm{spec}(\widetilde{A})$.
ii) λ *is of algebraic multiplicity* m.
iii) λ *is of geometric multiplicity 1.*
iv) $\widetilde{A}y = \lambda y$.

Remark. By property *iii)* the eigenvector y of $\widetilde{A}$ to λ is unique up to scaling. Note that y was an arbitrarily chosen eigenvector of A.

Proof. Let $Q^H AQ = D + N$ be the Schur decomposition for diagonal D, strictly upper triangular N and unitary Q [2, Theorem 7.1.3], where D_{ii} are the eigenvalues of A. We are free to assume the first column Q_1 of Q to be equal to $y/\|y\|$, and to assume $D_{11} = \ldots = D_{mm} = \lambda$. Then $A\overline{Q} = \overline{Q}(\lambda I_m + \overline{N})$ where $\overline{Q}$ comprises of the first m columns of Q and $\overline{N} \in M_m(\mathbb{IR})$ is strictly upper triangular. Based on $\overline{N}$ we define $\widehat{N} \in M_m(\mathbb{IR})$ by replacing all zero elements $\overline{N}_{i,i+1}$ in the first upper diagonal of $\overline{N}$ by some fixed ε. The geometric multiplicity of the m-fold eigenvalue λ of $\widehat{N}$ is equal to 1 because $\widehat{N}^{m-1} \neq 0$ [3, Section 3.2]. Denote by $\widetilde{N} \in M_n(\mathbb{IR})$ the strictly upper triangular matrix N with the left upper $m \times m$ matrix replaced by $\widehat{N}$. Then $\widetilde{A} := Q(D + \widetilde{N})Q^H$ has the same eigenvalues as A, the same Jordan structure as A except one $m \times m$ Jordan block for the eigenvalue λ, and y is a multiple of the first column of Q and henceforth an eigenvector of $\widetilde{A}$. The assertions are valid for every $\varepsilon > 0$, and this proves the lemma. ∎

Note that the Schur vectors of the new matrix $\widetilde{A}$ are the same as those of A, the eigenvectors are not. From this proof we do not get much insight how the eigenvectors change, in fact, how they "disappear" into $m-1$ principal vectors. To make this clear we give an

alternative proof of Lemma 2.1. Let $AS = SJ$ be a Jordan canonical form of A. Without loss of generality we may assume

$$J = \begin{pmatrix} J_{m_1}(\lambda) & & & & \\ & J_{m_2}(\lambda) & & & \\ & & \ddots & & \\ & & & J_{m_k}(\lambda) & \\ & & & & \ddots \end{pmatrix}$$

such that $J_{m_\nu}(\lambda),\ 1 \leq \nu \leq k$, are all Jordan blocks to λ and $\sum_{\nu=1}^{k} m_\nu = m$ [3, Section 3]. Here $J_p(\lambda)$ denotes a $p \times p$ Jordan block with main diagonal λ and first upper diagonal 1. Moreover, we may assume those blocks to be sorted by size: $m_1 \geq \ldots \geq m_k$. By assumption, y is an eigenvector of A, so it is a nontrivial linear

combination of those columns S_ν of S which are eigenvectors to λ : $y = \sum_{\nu=1}^{k} \alpha_\nu S_{q_\nu}$ with $q_\nu := 1 + \sum_{i=1}^{\nu-1} m_i$. Let α_p be the last of the nonzero coefficients α_ν, i.e. $\alpha_p \neq 0$ and $\alpha_\nu = 0$ for $p < \nu \leq k$. We define $T \in M_n(\mathbb{K})$ as follows:

$$T = \begin{pmatrix} I_{m_1} & & & \alpha_1 I_{m_1,m_p} & & & \\ & I_{m_2} & & \alpha_2 I_{m_2,m_p} & & & \\ & & \ddots & & & & \\ & & & \alpha_p I_{m_p} & & & \\ & & & & I_{m_{p+1}} & & \\ & & & & & \ddots & \end{pmatrix}.$$

Here $I_{r,s} \in M_{rs}(\mathbb{R})$ denotes the upper left submatrix with r rows and s columns of an identity matrix with $\max(r,s)$ rows and columns, $I_r := I_{r,r}$. So T is the identity matrix except the p-th block column, block sizes according to the Jordan canonical form of A. Then a little computation shows that $J_{m_\nu}(\lambda) \cdot \alpha_\nu I_{m_1,m_\nu} = \alpha_\nu I_{m_1,m_\nu} \cdot J_{m_\nu}(\lambda)$ and therefore J and T commute: $JT = TJ$. But T is constructed such that the eigenvector column of ST to the p-th block, i.e. the q_p-th column, is equal to y. Moreover, $\alpha_p \neq 0$ implies T to be nonsingular so that $A \cdot ST = ST \cdot J$ is a Jordan canonical form of A with the matrix ST comprising of the eigenvectors and principal vectors according to J, and the column q_p of ST being equal to y. Denote the permutation matrix permuting the blocks $(m_1, \ldots, m_p)$ of J into $(m_p, m_1, \ldots, m_{p-1})$ by P. Then $PAP^T \cdot PSTP^T = PSTP^T \cdot PJP^T$ is a Jordan canonical form of $\overline{A} := PAP^T$ with the first column of the eigenvector/principal vector basis $\overline{S} := PSTP^T$ being equal to y. Up to now we have a Jordan canonical form $\overline{A} \cdot \overline{S} = \overline{S} \cdot \overline{J}$ where $\overline{J} := PJP^T$ comprises of the Jordan blocks $J_{m_p}(\lambda), J_{m_1}(\lambda), \ldots, J_{m_{p-1}}(\lambda), \ldots, J_{m_k}(\lambda), \ldots$ and the first column of $\overline{S}$ is equal to y. Now change $\overline{J}$ into $\widetilde{J}$ by connecting all Jordan blocks belonging to λ by some $\delta \neq 0$ into one (Jordan) block to λ. The corresponding matrix $\widetilde{A}(\delta) = \widetilde{A} := \overline{S}\widetilde{J}\overline{S}^{-1}$ has an eigenvalue λ of algebraic multiplicity $m = \sum m_\nu$ and of geometric multiplicity 1 with corresponding eigenvector y, so it satisfies conditions $i)$ and $iv)$.

Remark. Note that the standard Jordan canonical form of $\widetilde{A}(\delta)$ can be obtained from $\overline{s}$ and $\widetilde{J}$ by a well known diagonal transformation. Note also that this transformation leaves the first column of $\overline{s}$, namely y, invariant but changes the other eigenvectors and principal vectors to λ significantly.

Since $\delta \neq 0$ is chosen arbitrary the distance $\|\widetilde{A} - \overline{A}\|$ can be made arbitrarily small, and $P^T \widetilde{A} P$ with the same spectral properties as $\widetilde{A}$ is arbitrarily close to A. This proves the lemma. ∎

We note that the constructed matrix T is a member of the larger class $\mathcal{T}$ of matrices defined as follows. All $T \in \mathcal{T}$ are upper triangular with the same block structure as J, the individual (upper diagonal) blocks being upper triangular Toeplitz. Those matrices $T \in \mathcal{T}$ form the set of matrices commuting with J [13]. The lemma above is the key to our main result for the general (non-symmetric) case.

THEOREM 2.2. *Let a predicate Φ be given such that Assumption 1.1 is satisfied, let $A \in M_n(\mathbb{K})$, closed $\Lambda \subseteq \mathbb{K}$, $X \subseteq \mathbb{K}^n$ and an ε-neigbourhood $U_\varepsilon(A)$ be given. Suppose the predicate $\Phi(\widetilde{A}, \Lambda, X)$ is satisfied for all $\widetilde{A} \in U_\varepsilon(A)$. This implies $\Phi(A, \Lambda, X)$ is satisfied and therefore existence of $\widehat{\lambda} \in \Lambda$, $0 \neq \widehat{x} \in X$ with $A\widehat{x} = \widehat{\lambda}\widehat{x}$. Suppose the eigenvalue $\widehat{\lambda}$ of A is unique in Λ, i.e. $\lambda \in \operatorname{spec}(A) \cap \Lambda \Rightarrow \lambda = \widehat{\lambda}$. Then for every eigenvector y of A to $\widehat{\lambda}$ there exists $0 \neq \alpha \in \mathbb{K}$ with $\alpha y \in X$.*

Remark. Note that the assertions in Assumption 1.1 are weak in the sense that only *existence* of an eigenvalue $\lambda \in \Lambda$ is asserted. Therefore we can obtain a result of the quality of Theorem 2.2 only in case Λ separates a multiple eigenvalue of A from the rest of the spectrum.

Proof. Let $0 \neq y \in \mathbb{K}^n$ be given with $Ay = \widehat{\lambda}y$. By Lemma 2.1 for every $\varepsilon > 0$ there exists $\widetilde{A} \in U_\varepsilon(A)$ such that y is (up to normalization) the unique eigenvector of $\widetilde{A}$ to $\widehat{\lambda}$. By assumption, $\widehat{\lambda}$ is the unique eigenvalue of A in Λ. Because Λ is closed and continuity of eigenvalues we may choose $\widetilde{A}$ close enough to A such that

$\widehat{\lambda}$ is the unique eigenvalue of $\widetilde{A}$ in Λ. By Assumption 1.1 this implies existence of an eigenvector $\widehat{y}$ of $\widetilde{A}$ to $\widehat{\lambda}$ in X, and $\widehat{y}$ must be a multiple of y. ∎

The practical interpretation is as follows. Suppose A has a multiple eigenvalue λ of geometric multiplicity $g > 1$, and λ is separated in Λ from the rest of the spectrum of A. Then an inclusion X must be large enough such that for every eigenvector y of A to λ a multiple of y must be in X. For eigenvectors normed to Euclidean norm 1 and $g = 2$, for example, X must contain a half circle closed at one end. For X being closed this implies $\mathcal{O} \in X$. However, a set X containing the zero vector seems not a desired inclusion for an eigenvector.

The same interpretation holds true if A has a cluster of m eigenvalues separated in Λ from the rest of spec(A), and there is some $\widetilde{A}$ nearby A with m-fold eigenvalue of geometric multiplicity greater than one.

We mention that one may feel uncomfortable with the above statements for the following reason. Let λ be an eigenvalue of geometric and algebraic multiplicity m. By the methods described in [10] we may find an inclusion $X \in \mathbb{I}M_{n,m}(\mathbb{K})$ for an invariant subspace of A. Every vector $\sum \alpha_\nu X_\nu$, X_i denoting the i-th column of X, is an eigenvector inclusion, so especially X_1. In such an argument an inherent discontinuity has been removed by assuming the geometric multiplicity to be equal to m. This is because a geometric multiplicity > 1 of an eigenvalue depends discontinuously on the matrix entries. The exact geometric multiplicity can only be computed if no rounding error whatsoever occurs, i.e. if all computations are exact.

For the same reason, narrow eigenvector inclusions seem only possible in case of exact computations. This is basically the assertion of Theorem 2.2.

3. Normal, Hermitian and symmetric matrices. Our assertions so far imply especially for symmetric matrices that narrow inclusions for a single eigenvector are not likely in case of a multiple or nearly multiple eigenvalue because algebraic and geometric multiplicity coincide for diagonalizable matrices. However, Theorem 2.2 constructs in general an *unsymmetric* matrix $\widetilde{A}$ in the neighbourhood of A with certain properties. Things might change if attention is restricted to symmetric, or more general, to Hermitian or normal matrices. However, the next theorem shows that this is not the case.

THEOREM 3.1. *Let a predicate Φ be given such that Assumption 1.1 is satisfied, let normal $A \in M_n(\mathbb{K})$, $\Lambda \subseteq \mathbb{K}$ and $X \subseteq \mathbb{K}^n$ be given. For given $\varepsilon > 0$ suppose the predicate $\Phi(\widetilde{A}, \Lambda, X)$ is satisfied for all normal matrices $\widetilde{A}$ with $\|\widetilde{A} - A\| < \varepsilon$. Denote by $\lambda_1, \ldots, \lambda_m$ all eigenvalues of A in Λ and denote by $x_1, \ldots, x_m$ the corresponding eigenvectors. Assume $\max_i |\lambda_i - \lambda| < \varepsilon$ for some given $\lambda \in \mathbb{K}$. Then for every orthogonal basis $y_1, \ldots, y_m$ of span$(x_1, \ldots, x_m)$ a multiple of at least one basis vector y_i lies in X, i.e. $\exists\, 0 \neq \alpha \in \mathbb{R} : \alpha y_i \in X$ for some $i \in \{1, \ldots, m\}$.*

Proof. Let $A = Q(\mathrm{diag}(\lambda_1, \ldots, \lambda_m) \oplus D)Q^H$ be the eigendecomposition of A for unitary Q and diagonal $D \in M_n(\mathbb{K})$. Let $Q = [U\ V]$ be the splitting of Q into its first m and following $n-m$ columns. The columns of U are multiples of $x_1, \ldots, x_m$ and there is unitary $W \in M_m(\mathbb{K})$ such that the columns of $UW \in M_{n,m}(\mathbb{K})$ are scalar multiples of $y_1, \ldots, y_m$. Denote $\widetilde{A} := [UW\ V](\lambda I_m \oplus D)[UW\ V]^{-1}$. Then

$$\begin{aligned} \|\widetilde{A} - A\| &= \|UW \cdot \lambda I_m \cdot W^H U^H - U\,\mathrm{diag}(\lambda_1, \ldots, \lambda_m)U^H\| \\ &= \|\lambda \cdot UU^H - U\,\mathrm{diag}(\lambda_1, \ldots, \lambda_m)U^H\| \\ &= \max|\lambda - \lambda_i| < \varepsilon, \end{aligned}$$

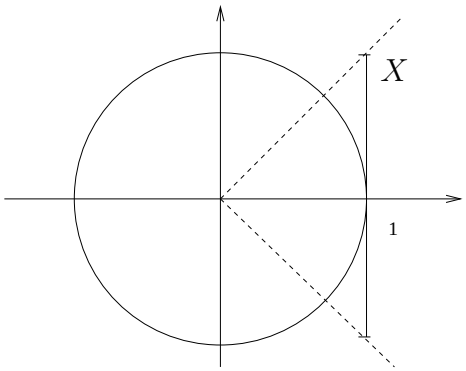
the last inequality by the definition of λ. Therefore the predicate $\Phi(\widetilde{A}, \Lambda, X)$ is satisfied, and since λ is the only eigenvalue of $\widetilde{A}$ in Λ the theorem follows. ∎

Remark. In a practical application λ may be chosen to be the center of the smallest circle containing all λ_i.

The proof of Theorem 3.1 is easily adapted to special cases such as Hermitian, symmetric or skewsymmetric matrices. In the symmetric case, the sets Λ and X can be real, and unitary Q in the proof means orthogonal. For its importance, we repeat this special case in a corollary.

COROLLARY 3.2. *Let a predicate Φ be given such that Assumption 1.1 is satisfied, let $A \in M_n(\mathbb{R})$, $A^T = A$, $\Lambda \subseteq \mathbb{R}$ and $X \subseteq \mathbb{R}^n$ be given. For given $\varepsilon > 0$ suppose the predicate $\Phi(\widetilde{A}, \Lambda, X)$ is satisfied for all $\widetilde{A}^T = \widetilde{A}$ with $\|\widetilde{A} - A\| < \varepsilon$. Denote by $\lambda_1, \ldots, \lambda_m$ all eigenvalues of A in Λ and denote by $x_1, \ldots, x_m$ the corresponding eigenvectors. Assume $\max_{i,j} |\lambda_i - \lambda_j| < 2\varepsilon$. Then for every orthogonal basis $y_1, \ldots, y_m$ of span$(x_1, \ldots, x_m)$ a multiple of at least one basis vector y_i lies in X, i.e. $\exists 0 \neq \alpha \in \mathbb{R} : \alpha y_i \in X$ for some $i \in \{1, \ldots, m\}$.*

The interpretation of Corollary 3.2 is as follows. Let a symmetric matrix be given with more than one eigenvalue in Λ, say λ_1 and λ_2. Those eigenvalues must be clustered, otherwise one could just wide Λ to cover more eigenvalues and nothing could be deduced. Then eigenvector inclusions must be wide enough to cover a suitable multiple of at least one basis vector of *every* orthogonal basis (y_1, y_2) of span(x_1, x_2). For normalization of eigenvectors $\|x\|_2 = 1$ this means that



an interval inclusions must cover at least an angle of 90° as in the picture above. So narrow inclusions seem not likely to be possible. The only exception to this statement would be one wide inclusion covering X in order to satisfy Theorem 3.1 and other narrow inclusions covering other eigenvectors. This seems not likely to be possible. The theorem above has, of course, an obvious generalization to the Hermitian and normal case.

In the m-dimensional case with eigenvectors normed to Euclidean norm 1 this means the following. The m unit vectors define an m-dimensional ball with radius $\sqrt{1 - 1/m}$. Hence the diameter of X, i.e. $\{\max \|x_1 - x_2\| : x_1, x_2 \in X\}$ cannot be smaller than $2\sqrt{1 - 1/m}$, otherwise we would find m orthogonal unit vectors not contained in X. In other words, the relative error of the inclusion X is near 1.

4. Geometric multiplicity one. The question remains whether eigenvector inclusions are possible in case of geometric multiplicity one of the eigenvalue λ. In this case there is one Jordan block to λ and, up to normalization, a unique eigenvector. For $B \in M_n(\mathbb{K})$, consider the adjugate of classical adjoint matrix adj(B) defined by

$$[\mathrm{adj}(B)]_{ij} := (-1)^{i+j} \det B(j,i)$$

(cf. [3], [4]), where $B(j,i) \in M_{n-1}(\mathbb{K})$ denotes the matrix B without j-th row and i-th column. Then $B \cdot \mathrm{adj}B = \det B \cdot I$, and therefore

$$(A - \lambda I) \cdot \mathrm{adj}(A - \lambda I) \equiv 0. \tag{1}$$

That means, as is well known, every nonzero column of adj$(A - \lambda I)$ is an eigenvector of A to λ. In case of λ being of geometric multiplicity 1 an eigenvector may be computed by some well known determinantal calculations as follows. By assumption, the dimension of the kernel of $A - \lambda I$ is 1, hence rank(adj$(A - \lambda I)) \leq 1$. The elements of adj$(A - \lambda I)$ are the $(n-1) \times (n-1)$ minors of $A - \lambda I$. Not all of them can be zero because then rank$(A - \lambda I) \leq n - 2$. Therefore rank(adj$(A - \lambda I)) = 1$, and there exists at least one nonzero column. By (1), this is an eigenvector to the eigenvalue λ.

It remains to compute verified error bounds. Of course, this can be done by computing n bounds for $(n-1)\times(n-1)$ determinants, but one can do better.

For given λ let $\widetilde{x}$ be an approximation to the eigenvector of λ. Note that we also have to prove that the geometric multiplicity of λ is indeed 1. Let $|x_k| = \max|\widetilde{x}_i|$. We try to find an inclusion of the solution of the overdetermined system

$$\begin{aligned}(A-\lambda I)y &= 0\\ e_k^T y &= 1.\end{aligned} \tag{2}$$

These are $n+1$ equations in the n unknowns y_i. Given an inclusion Λ of an eigenvalue λ of A, the following theorem tells how to compute an inclusion of the corresponding eigenvector. It includes the proof that the geometric multiplicity of λ is 1. Note that the methods in [1] and [10] allow computation of an inclusion of an invariant subspace to λ but not of an individual eigenvector.

In order to open the follwoing theorem for a practical comutation we assume set quantities to be intervals, interval vectors or interval matrices. denoted by $\mathbb{IIK}$, $\mathbb{IIK}^n$ and $\mathbb{I}M_n(\mathbb{K})$, respectively. For details cf. [8].

THEOREM 4.1. *Let $\mathbb{K}\in\{\mathbb{R},\mathbb{C}\}$ and $A\in M_n(\mathbb{K})$ be given, and let $\mathbf{\Lambda}\in\mathbb{IIK}$ be an inclusion of an eigenvalue of A. Denote by $I^{(i)}\in M_{n-1,n}$ the $n\times n$ identity matrix I without i-th row, and denote by $J^{(k)}\in M_{n,n-1}$ the $n\times n$ identity matrix without k-th column. Denote the k-th column of I by e_k. For fixed $i,k\in\{1,\ldots,n\}$ define $\mathbf{B}\in\mathbb{I}M_{n-1}(\mathbb{K})$ by $\mathbf{B}:=I^{(i)}(A-\mathbf{\Lambda}I)J^{(k)}$, and define $\mathbf{b}\in\mathbb{IIK}^{n-1}$ by $\mathbf{b}:=-I^{(i)}(A-\mathbf{\Lambda}I)e_k$. Let $\mathbf{Z}\in I\mathbb{K}^{n-1}$ be given such that*

$$\sum(\mathbf{B},\mathbf{b}) = \{z\in\mathbb{K}^{n-1}:\ \exists\ \widetilde{B}\in\mathbf{B},\exists\,\widetilde{b}\in\mathbf{b},\ \widetilde{B}z=\widetilde{b}\}\subseteq\mathbf{Z},$$

and assume every $\widetilde{B}\in\mathbf{B}$ to be nonsingular. Then the following holds true:

i) Every eigenvalue λ of A with $\lambda\in\mathbf{\Lambda}$ has geometric multiplicity one.
ii) To every such eigenvalue λ, $\mathbf{X}=(\mathbf{Z}_1,\ldots,\mathbf{Z}_{k-1},1,\mathbf{Z}_k,\ldots,\mathbf{Z}_{n-1})^T\in\mathbb{IIK}^n$ is an inclusion of the corresponding eigenvector.

Proof. Let $\lambda\in\mathbf{\Lambda}$ be a fixed but arbitrary eigenvalue of A, so $\mathrm{rank}(A-\lambda I)\le n-1$. By definition, $\mathbf{B}$ is an inclusion of an $(n-1)\times(n-1)$ submatrix of $A-\lambda I$. Then $\mathrm{rank}(A-\lambda I)\ge n-1$ because $\mathbf{B}$ is nonsingular. Therefore the geometric multiplicity of λ is 1 and $\mathrm{rank}(A-\lambda I)=n-1$. By assumption, the solution z of

$$I^{(i)}(A-\lambda I)J^{(k)}\cdot z = -I^{(i)}(A-\lambda I)e_k$$

is included in $\mathbf{Z}$. Defining $x:=(z_1,\ldots,z_{k-1},1,z_k,\ldots,z_{n-1})^T\in\mathbb{K}^n$ and rearranging shows

$$I^{(i)}(A-\lambda I)x = 0,$$

that means $[(A-\lambda I)x]_\nu = 0$ for $1\le\nu\le n$, $\nu\ne i$. But $\mathrm{rank}(A-\lambda I)=\mathrm{rank}(I^{(i)}(A-\lambda I))=n-1$, so the i-th row of $A-\lambda I$ is linear dependent of the others. Therefore, $(A-\lambda I)x=0$, and $0\ne x\in\mathbf{X}$ proves the theorem. ■

In view of the discussion after Theorem 4.1 note that the property of an eigenvalue that its geometric multiplicity is one depends continuously on the matrix entries, i.e. it remains constant. This is only true for geometric multiplicity one.

For a practical application, the column k may be chosen as before by $|\widetilde{x}_k| = \max|\widetilde{x}_\nu|$. The row i should be picked such that $I^{(i)}(A-\Lambda I)J^{(k)}$ is far from singularity. For this we perform an LU-decomposition of $A-\mathrm{mid}(\Lambda)\cdot I$ with partial pivoting. In exact computation with $\mathrm{mid}(\Lambda)$ being an exact eigenvalue of A with geometric multiplicity one, this yields a singular factor U with $U_{\nu\nu}\ne 0$ for $1\le\nu\le n-1$ and $U_{nn}=0$. We define i to be the index of the row which is treated last in the LU-decomposition due to partial pivoting. Note that the method works only as long as nearby matrices with multiple eigenvalues have only such with geometric multiplicity one. Computing Z by some self-validating method (see [8] or [11], where the latter

is the introduction to the LAA special issue on self-validating methods) proves nonsingularity of B, so all assumptions of the theorem can be verified on the computer. A standard Matlab implementation `verifylss` of such an algorithm can be found in [9].

Note that if A has a m-fold multiple eigenvalue of geometric multiplicity one, then in every ε-neighbourhood of A there are matrices with m simple eigenvalues. By the theorem, all corresponding eigenvectors are enclosed in Z. This assures again the well known fact that in such a case those eigenvectors are almost linear dependent. Also note that the assumption $\Lambda \cap \mathrm{spec}(A) \neq \emptyset$ is necessary, that means the theorem cannot be used to validate existence of an eigenvalue $\lambda \in \Lambda$.

5. Computational results. Some computational results are generated as follows. For given n and m we generate

$$J = \begin{pmatrix} 2 & 1 & & & & & & & \\ & 2 & 1 & & & & & & \\ & & \ddots & \ddots & & & & & \\ & & & \ddots & 1 & & & & \\ & & & & 2 & & & & \\ & & & & & r_1 & & & \\ & & & & & & r_2 & & \\ & & & & & & & \ddots & \\ & & & & & & & & r_{n-m} \end{pmatrix}$$

with r_i, $1 \leq i \leq m-n$, randomly picked in $[-1,1]$ with uniform distribution, and m diagonal entries 2. So J has a $m \times m$ Jordan block to the eigenvalue 2. This eigenvalue 2 is sufficiently separated from the other eigenvalues of J. We generate $X \in M_n(\mathbb{R})$ randomly and define $A := XJX^{-1}$. The latter computation uses floating point operations, so that up to rounding errors A should be not too far from a matrix with m-fold eigenvalue 2 and geometric multiplicity 1.

We then calculate eigenvector/eigenvector approximations of A by the Matlab routine `eig` [5], and based on these approximations we calculate an inclusion $\Lambda \in \mathbb{IC}$ of the m-fold eigenvalue 2 by the methods described in [10].

Based on this inclusion Λ we use the method described in Theorem 4.1 to calculate an inclusion X of the corresponding eigenvector. Note that this includes the proof that the geometric multiplicity of every eigenvalue in Λ is indeed equal to one. The indices k and i are computed as described before.

Computations are performed in INTLAB [9] in double precision. This is a public domain Matlab toolbox with easy operator-like access to interval operations, standard functions, automatic differentiation and more. For different values of n and m we ran 100 test cases each and display the median of relative errors of the inclusion interval vectors X and the eigenvalue sensitivity $\varepsilon^{1/m}$.

In the second last column the number Λ-failed gives the number of samples (out of 100) where inclusion of the eigenvalue failed. For increasing n and especially increasing values of m the inclusion becomes more and more difficult due to the increasing sensitivity of the eigenvalue of geometric multiplicity one. In the last column, the number X-failed is the number of test cases where inclusion of the eigenvector failed (of course, only if inclusion of Λ succeeded). In our test cases this never happened.

n	m	median relative error	$\varepsilon^{1/m}$	Λ-failed	X-failed
20	2	7.5e-9	1.5e-8	0	0
	3	4.6e-9	6.1e-6	0	0
	4	1.1e-4	1.2e-4	3	0
	5	8.4e-4	7.4e-4	9	0
50	2	3.3e-8	1.5e-8	17	0
	3	2.4e-5	6.1e-6	4	0
	4	5.0e-4	1.2e-4	8	0
	5	4.2e-3	7.4e-4	33	0
100	2	2.2e-7	1.5e-8	11	0
	3	1.6e-4	6.1e-6	5	0
	4	4.2e-3	1.2e-4	22	0
	5	2.3e-2	7.4e-4	80	0
200	2	7.0e-6	1.5e-8	4	0
	3	3.0e-3	6.1e-6	10	0
	4	4.3e-2	1.2e-4	96	0
	5	-	7.4e-4	100	0

The accuracy of the inclusion X of the eigenvector is determined by the accuracy of the inclusion of Λ and henceforth by the algebraic multiplicity m of the eigenvalue $\lambda = 2$. Note the correspondence of the median relative error of X and the eigenvalue sensitivity $\varepsilon^{1/m}$, ε denoting the relative rounding error unit.

For larger size of the Jordan block the eigenvalue becomes very sensitive to perturbations in the matrix A. That means the inclusion Λ is of poorer quality with increasing algebraic multiplicity of λ whilest geometric multiplicity one, that is the diameter of the diagonal elements of $A - \Lambda I$ increases and henceforth the quality of the inclusion of the eigenvector decreases.

To test the quality of the eigenvector inclusion for better inclusions Λ we constructed examples with *precisely* the Jordan structure as above, that is an exactly m-fold eigenvalue 2 with geometric multiplicity 1. The inclusion Λ is therefore the point interval 2. The corresponding results are in the table below. We see the mild dependency on the dimension of the matrix, but inclusions seem insensitive to the algebraic multiplicity, even for extreme cases as an 20-fold eigenvalue.

		relative error of X			
n	m	median	maximum	$\varepsilon^{1/m}$	X-failed
50	2	2.9e-14	3.6e-12	1.5e-8	0
	5	2.7e-14	4.0e-12	7.4e-4	0
	10	2.2e-14	2.6e-12	2.7e-2	0
	20	1.5e-14	1.6e-12	1.6e-1	0
100	2	1.3e-13	2.7e-11	1.5e-8	0
	5	1.2e-13	2.7e-11	7.4e-4	0
	10	1.1e-13	2.3e-11	2.7e-2	0
	20	9.5e-14	1.8e-11	1.6e-1	0
200	2	5.1e-13	2.0e-10	1.5e-8	0
	5	5.0e-13	2.0e-10	7.4e-4	0
	10	4.9e-13	1.7e-10	2.7e-2	0
	20	4.9e-13	1.4e-10	1.6e-1	0

Finally we reproduce the matrix $\widetilde{A}(\delta)$ in the second proof of Lemma 2.1 to demonstrate the sensitivity of the eigenvector by transforming δ into 1. Let A be a 100×100 matrix with two Jordan blocks of size m, both to the eigenvalue 2, and $100 - 2m$ randomly chosen simple eigenvalues between -1 and 1. For $A = SJS^{-1}$ denote by $\widetilde{J}$ the Jordan matrix with the two $m \times m$ blocks connected by δ, i.e. $\widetilde{J}_{ij} = J_{ij}$ except

$\widetilde{J}_{m,m+1} := \delta$, and denote $\widetilde{A}(\delta) := S\widetilde{J}S^{-1}$. Decreasing δ makes the linear system in Theorem 4.1 more and more ill-conditioned, as can be seen from the following table.

		relative error of X		
m	δ	median	maximum	X-failed
2	10^{-2}	2.1e-13	2.8e-12	0
5	10^{-2}	2.1e-13	8.8e-11	0
2	10^{-6}	2.1e-9	2.7e-8	0
5	10^{-6}	2.5e-9	5.4e-7	0
2	10^{-12}	2.2e-3	2.6e-2	0
5	10^{-12}	2.3e-3	9.8e-2	0
2	10^{-13}	3.1e-2	9.0e-1	3
5	10^{-13}	2.8e-2	1.7e0	2

Again we performed 100 test cases each. As expected the product of δ and the relative error of the inclusion X is of the order of the relative rounding error unit ε. For $\delta = 10^{-14}$ and less no inclusion was possible.

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