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JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
Journal of Computational and Applied Mathematics 167 (2004) 493–498
www.elsevier.com/locate/cam

An analogue of the results of Saad and Stewart for harmonic Ritz vectors☆

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Received 1 May 2003; received in revised form 14 October 2003

Abstract

Let (λ, x) be an eigenpair of the matrix A of order n and let (μ, u) be a Ritz pair of A with respect to a subspace $\mathscr{K}$. Saad has derived a simple priori error bound for $\sin\angle(x,u)$ in terms of $\sin\angle(x,\mathscr{K})$ for A Hermitian. Similar to Saad's result, Stewart has got an equally simple inequality for A non-Hermitian. In this paper, let (θ, w) be a harmonic Ritz pair from a subspace $\mathscr{K}$, a similar priori error bound for $\sin\angle(x,w)$ is established in terms of $\sin\angle(x,\mathscr{K})$.

MSC: 15A18; 65F15

Keywords: Eigenproblem; Harmonic Rayleigh–Ritz method; Harmonic Ritz vector

1. The results of Saad and Stewart

Throughout the paper, the eigenvectors and the approximate eigenvectors are normalized to have unit length. The norm used is the Euclidean norm. Denote by the superscript H the conjugate transpose of a matrix or vector.

Let A be a large matrix of order n. Given a subspace $\mathscr{K}$, the Rayleigh–Ritz method extracts approximations to some eigenpairs (λ, x) of A with respect to $\mathscr{K}$ by computing the so called Ritz

☆ Supported by the Special Funds (G1999032805).
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0377-0427/$ - see front matter
doi:10.1016/j.cam.2003.10.020

pairs (μ, u) that satisfy the conditions

$$u \in \mathscr{K},$$

$$Au - \mu u \perp \mathscr{K}. \tag{1}$$

It is easy to verify that if K is an orthonormal basis for $\mathscr{K}$ then the Ritz vectors $u = Ky$, where the (μ, y) are the solutions of the eigenproblem $K^{\mathrm{H}}AKy = \mu y$.

Saad [1, Theorem 4.6] has established the following a priori error bound for u.

Theorem 1. *Let (μ, u) be a Ritz pair of the Hermitian matrix A with respect to the subspace $\mathscr{K}$. Let $P_{\mathscr{K}}$ be the orthogonal projector on $\mathscr{K}$, and for a nonzero vector v define*

$$\angle(v, \mathscr{K}) = \min_{w \in \mathscr{K}, w \neq 0} \angle(v, w).$$

Then

$$\sin\angle(x, u) \leqslant \sin\angle(x, \mathscr{K}) \sqrt{1 + \frac{\gamma^2}{\delta^2}}, \tag{2}$$

where

$$\gamma = \|P_{\mathscr{K}} A (I - P_{\mathscr{K}})\|$$

and δ is the distance between λ and the Ritz values other than μ.

Recently, Stewart [3] has extended the above result to the non-Hermitian case in the following way.

Theorem 2. *Assume that (μ, u) is a Ritz pair of the matrix A with respect to the subspace $\mathscr{K}$ and that the matrix V having orthonormal columns spans the orthogonal complement of u with respect to $\mathscr{K}$. Define $G = V^{\mathrm{H}}AV$ and*

$$\operatorname{sep}(\lambda, G) = \min_{\|z\|=1} \|Gz - \lambda z\|.$$

Then

$$\sin\angle(x, u) \leqslant \sin\angle(x, \mathscr{K}) \sqrt{1 + \frac{\gamma^2}{\operatorname{sep}(\lambda, G)^2}}. \tag{3}$$

2. The harmonic Rayleigh–Ritz method

Suppose that we want to compute a few eigenvalues of A near a target point τ in the complex plane and that factoring $(A - \tau I)^{-1}$ is too expensive and even impractical. An usual procedure for doing this is the harmonic Rayleigh–Ritz method [2]. The approximate eigenpair (θ, w) computed by the harmonic Rayleigh–Ritz method is called the harmonic Ritz pairs. We now extend the above results of Saad and Stewart to the harmonic Rayleigh–Ritz method. We establish a priori error bound for $\sin\angle(x, w)$ in terms of $\sin\angle(x, \mathscr{K})$ for harmonic Rayleigh–Ritz method.

The harmonic Rayleigh–Ritz method extracts approximations to some eigenvalues λ near a target point τ of A and the corresponding eigenvectors with respect to $\mathscr{K}$ by computing the so-called harmonic Ritz pairs (θ, w) that satisfy the conditions

$$w \in \mathscr{K},$$
$$Aw - \theta w \perp (A - \tau I)\mathscr{K}. \tag{4}$$

Assume that $K^{\mathrm{H}}(A-\tau I)^{\mathrm{H}}K$ is invertible. Then it is easy to verify that if K is an orthonormal basis for $\mathscr{K}$, $w = Ky$ where the (θ, y) are the solutions of the eigenproblem

$$(K^{\mathrm{H}}(A-\tau I)^{\mathrm{H}}K)^{-1}K^{\mathrm{H}}(A-\tau I)^{\mathrm{H}}(A-\tau I)Ky = (\theta - \tau)y.$$

Without loss of generality, in the sequel, we suppose for brevity that $\tau = 0$. The above relation reduces to

$$(K^{\mathrm{H}}A^{\mathrm{H}}K)^{-1}K^{\mathrm{H}}A^{\mathrm{H}}AKy = \theta y. \tag{5}$$

3. A priori error bound for *w*

First we give a lemma.

Lemma 1. *Let (w, V) be a column orthonormal matrix in which the columns of V span the orthogonal complement of the harmonic Ritz vector w with respect to $\mathscr{K}$. Define*

$$B = \begin{pmatrix} w^{\mathrm{H}} \\ V^{\mathrm{H}} \end{pmatrix} A^{\mathrm{H}}(w \ \ V), \quad C = \begin{pmatrix} w^{\mathrm{H}} \\ V^{\mathrm{H}} \end{pmatrix} A^{\mathrm{H}}A(w \ \ V), \tag{6}$$

and assume that B is invertible. Then the eigenvalues of the matrix $B^{-1}C$ are the harmonic Ritz values of A with respect to $\mathscr{K}$ and

$$B^{-1}C = \begin{pmatrix} \theta & G_1 \\ 0 & G \end{pmatrix},$$

where G is an $(m-1)\times(m-1)$ matrix whose eigenvalues are the harmonic Ritz values other than θ.

Proof. If K is an orthonormal basis for $\mathscr{K}$, there exists a unitary matrix Q such that

$$K = (w, V)Q.$$

Then the harmonic Ritz values of A with respect to $\mathscr{K}$ are the eigenvalues of the matrix

$$\begin{aligned}(K^{\mathrm{H}}A^{\mathrm{H}}K)^{-1}K^{\mathrm{H}}A^{\mathrm{H}}AK &= \left(Q^{\mathrm{H}}\begin{pmatrix} w^{\mathrm{H}} \\ V^{\mathrm{H}} \end{pmatrix} A^{\mathrm{H}}(w, V)Q\right)^{-1} Q^{\mathrm{H}}\begin{pmatrix} w^{\mathrm{H}} \\ V^{\mathrm{H}} \end{pmatrix} A^{\mathrm{H}}A(w, V)Q \\ &= (Q^{\mathrm{H}}BQ)^{-1}Q^{\mathrm{H}}CQ \\ &= Q^{\mathrm{H}}B^{-1}CQ.\end{aligned}$$

According to (4), we have

$$w^{\mathrm{H}}A^{\mathrm{H}}Aw=\theta w^{\mathrm{H}}A^{\mathrm{H}}w, \quad V^{\mathrm{H}}A^{\mathrm{H}}Aw=\theta V^{\mathrm{H}}A^{\mathrm{H}}w.$$

So

$$C=\begin{pmatrix}\theta w^{\mathrm{H}}A^{\mathrm{H}}w & w^{\mathrm{H}}A^{\mathrm{H}}AV\\ \theta V^{\mathrm{H}}A^{\mathrm{H}}w & V^{\mathrm{H}}A^{\mathrm{H}}AV\end{pmatrix}.$$

Let $B^{-1}C=Y=\begin{pmatrix}Y_1 & Y_2\\ Y_3 & Y_4\end{pmatrix}$, i.e., $BY=C$. Then it is easily verified that $Y_1=\theta,\ Y_3=0$ is a solution of the matrix equation $BY=C$. Since B is supposed to be nonsingular, Y is uniquely determined. □

Having the lemma, we can now present our main result.

Theorem 3. *Let (θ,w) be a harmonic Ritz pair with respect to the subspace $\mathscr{K}$. Then*

$$\sin\angle(x,w)\leqslant\sin\angle(x,\mathscr{K})\sqrt{1+\frac{\gamma_1^2\|B^{-1}\|^2}{\mathrm{sep}(\lambda,G)^2}}, \tag{7}$$

where $\gamma_1=\|P_{\mathscr{K}}A^{\mathrm{H}}(\lambda I-A)(I-P_{\mathscr{K}})\|$ and the matrix G is as defined in Lemma 1.

Proof. Assume that W is such that (w,V,W) is unitary. Let

$$x=(w\ \ V\ \ W)\begin{pmatrix}z_1\\ z_2\\ z_3\end{pmatrix}. \tag{8}$$

Then by definition we have

$$\sin\angle(x,\mathscr{K})=\|W^{\mathrm{H}}x\|=\|z_3\|, \tag{9}$$

and

$$\sin\angle(x,w)=\|(V\ \ W)^{\mathrm{H}}x\|=\sqrt{\|z_2\|^2+\|z_3\|^2}. \tag{10}$$

From the relation $Ax=\lambda x$ we get

$$A^{\mathrm{H}}Ax=\lambda A^{\mathrm{H}}x.$$

Left multiplying both hand-sides by $\begin{pmatrix}w^{\mathrm{H}}\\ V^{\mathrm{H}}\\ W^{\mathrm{H}}\end{pmatrix}$ and using (8), we then get

$$\begin{pmatrix}w^{\mathrm{H}}\\ V^{\mathrm{H}}\\ W^{\mathrm{H}}\end{pmatrix}A^{\mathrm{H}}A(w\ \ V\ \ W)\begin{pmatrix}z_1\\ z_2\\ z_3\end{pmatrix}=\lambda\begin{pmatrix}w^{\mathrm{H}}\\ V^{\mathrm{H}}\\ W^{\mathrm{H}}\end{pmatrix}A^{\mathrm{H}}(w\ \ V\ \ W)\begin{pmatrix}z_1\\ z_2\\ z_3\end{pmatrix}.$$

Making use of relation (6) gives

$$\begin{pmatrix} C & C_1 \\ C_2 & C_3 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \lambda \begin{pmatrix} B & B_1 \\ B_2 & B_3 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix}$$

with $C_1 = \binom{w^H A^H A W}{V^H A^H A W}$ and $B_1 = \binom{w^H A^H W}{V^H A^H W}$. Therefore, we have

$$C \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} + C_1 z_3 = \lambda B \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} + \lambda B_1 z_3,$$

i.e.,

$$(B^{-1}C - \lambda I) \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = B^{-1}(\lambda B_1 - C_1) z_3.$$

By Lemma 1, we have

$$\begin{pmatrix} \theta - \lambda & G_1 \\ 0 & G - \lambda I \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = B^{-1}(\lambda B_1 - C_1) z_3. \tag{11}$$

The right-hand side of (11) can be bounded from above as follows:

$$\begin{aligned} \|B^{-1}(\lambda B_1 - C_1) z_3\| &\leqslant \|B^{-1}\| \|\lambda B_1 - C_1\| \|z_3\| \\ &\leqslant \|B^{-1}\| \|P_{\mathscr{K}} A^H (\lambda I - A)(I - P_{\mathscr{K}})\| \|z_3\| \\ &= \gamma_1 \|B^{-1}\| \|z_3\|. \end{aligned} \tag{12}$$

The left-hand side of (11) can be bounded from below as follows:

$$\begin{aligned} \left\| \begin{pmatrix} \theta - \lambda & G_1 \\ 0 & G - \lambda I \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \right\| &= \left\| \begin{pmatrix} (\theta - \lambda) z_1 + G_1 z_2 \\ (G - \lambda I) z_2 \end{pmatrix} \right\| \\ &\geqslant \|(G - \lambda I) z_2\| \\ &\geqslant \operatorname{sep}(\lambda, G) \|z_2\|. \end{aligned} \tag{13}$$

Combining (13) and (12), we have

$$\|z_2\| \leqslant \frac{\gamma_1 \|B^{-1}\|}{\operatorname{sep}(\lambda, G)} \|z_3\|. \tag{14}$$

It follows from (14), (9) and (10) that (7) holds. □

Theorem 3 is an exact analogue of Theorem 2 for the harmonic Rayleigh–Ritz method. The major difference is that the bound for $\sin(x, w)$ is now related to $\|B^{-1}\|$, besides $\sin(x, \mathscr{K})$ and $\operatorname{sep}(\lambda, G)$. While γ_1 is uniformly bounded with respect to $\mathscr{K}$, for a general A, there is no guarantee that $\|B^{-1}\|$ is uniformly bounded with respect to $\mathscr{K}$, so that the right-hand side of (7) may not approach zero as $\sin\angle(x, \mathscr{K}) \to 0$ and thus w may not converge to x. Furthermore, B may even be singular and $\|B^{-1}\|$ is thus infinitely large. This shows that a harmonic Ritz vector may be more difficult to converge than a Ritz vector.

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