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# A generalization of Saad's bound on harmonic Ritz vectors of Hermitian matrices



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## ABSTRACT

We prove a Saad's type bound for harmonic Ritz vectors of a Hermitian matrix. The new bound reveals a dependence of the harmonic Rayleigh–Ritz procedure on the condition number of a shifted problem operator. Several practical implications are discussed. In particular, the bound motivates incorporation of preconditioning into the harmonic Rayleigh–Ritz scheme.

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## 1. Introduction

The Rayleigh–Ritz procedure is a well known technique for approximating eigenpairs  $(\lambda, x)$  of an  $n$ -by- $n$  matrix  $A$  over a given subspace  $\mathcal{K}$  [9,11,15]. It produces approximate eigenpairs  $(\mu, u)$ , called the Ritz pairs, that satisfy the Galerkin condition

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$$Au - \mu u \perp \mathcal{K}, \quad u \in \mathcal{K}.$$

This is done by solving an  $s$ -by- $s$  eigenvalue problem

$$K^*AKc = \mu K^*Kc, \tag{1}$$

where  $K$  is a matrix whose columns contain a basis of  $\mathcal{K}$  and  $s = \dim(\mathcal{K}) \ll n$ . The eigenvalues  $\mu$  of the projected problem (1), called the Ritz values, represent approximations to the eigenvalues  $\lambda$  of  $A$ . The associated eigenvectors  $x$  are approximated by the Ritz vectors  $u = Kc$ .

For a Hermitian matrix  $A$ , a general a priori bound that describes the approximation quality of Ritz vectors is due to Saad [11, Theorem 4.6]. The bound shows that the proximity of a Ritz vector  $u$  to an exact eigenvector  $x$  is determined essentially by the angle between this eigenvector and the subspace  $\mathcal{K}$ , defined as

$$\angle(x, \mathcal{K}) = \min_{y \in \mathcal{K}, y \neq 0} \angle(x, y). \tag{2}$$

This result (in a slightly generalized form) is stated in Theorem 1.

**Theorem 1.** (See Saad [11].) *Let  $(\lambda, x)$  be an eigenpair of a Hermitian matrix  $A$  and  $(\mu, u)$  be a Ritz pair with respect to the subspace  $\mathcal{K}$ . Assume that  $\Theta$  is a set of all the Ritz values and let  $P_{\mathcal{K}}$  be an orthogonal projector onto  $\mathcal{K}$ . Then*

$$\sin \angle(x, u) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{K}), \tag{3}$$

where  $\gamma = \|P_{\mathcal{K}}A(I - P_{\mathcal{K}})\|$  and  $\delta$  is the distance between  $\lambda$  and the Ritz value other than  $\mu$ , i.e.,

$$\delta = \min_{\mu_j \in \Theta \setminus \mu} |\lambda - \mu_j|. \tag{4}$$

Throughout,  $\|\cdot\|$  denotes either the spectral or the Frobenius norm of a matrix; or a vector’s 2-norm, depending on the context. The matrix Frobenius norm will be denoted by  $\|\cdot\|_F$ .

Bound (3) is often referred to as “Saad’s bound” in literature, e.g., [2,16]. It was later extended by Stewart [16] to invariant subspaces of general matrices.

**Theorem 2.** (See Stewart [16].) *Let  $\mathcal{X}$  be an invariant subspace of a (possibly non-Hermitian) matrix  $A$ . Let  $\mathcal{U}$  be a Ritz subspace<sup>1</sup> and  $\mathcal{V}$  its orthogonal complement in  $\mathcal{K}$ . Then*

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<sup>1</sup> Let  $(M, U)$  be a matrix pair, such that all columns of  $U$  are in  $\mathcal{K}$  and  $AU - UM \perp \mathcal{K}$ . Then the Ritz subspace  $\mathcal{U} \subseteq \mathcal{K}$  is defined as a column space of  $U$ . If  $A$  is Hermitian, then  $\mathcal{U}$  is a subspace spanned by Ritz vectors.

$$\sin \angle(\mathcal{X}, \mathcal{U}) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(\mathcal{X}, \mathcal{K}), \tag{5}$$

with  $\gamma = \|P_{\mathcal{K}}A(I - P_{\mathcal{K}})\|$  and  $\delta$  defined by

$$\delta = \inf_{\|Z\|=1} \|(V^*AV)Z - Z(X^*AX)\|, \tag{6}$$

where  $X$  and  $V$  are arbitrary orthonormal bases of  $\mathcal{X}$  and  $\mathcal{V}$ , respectively.

The angle between two subspaces in (5) is defined as

$$\angle(\mathcal{X}, \mathcal{K}) = \min_{\substack{x \in \mathcal{X}, x \neq 0 \\ y \in \mathcal{K}, y \neq 0}} \angle(x, y). \tag{7}$$

Note that if  $A$  is Hermitian and  $\mathcal{X}, \mathcal{U}$  are one-dimensional subspaces spanned by an eigenvector  $x$  and a Ritz vector  $u$ , respectively, then the values of  $\delta$  in (4) and (6) coincide; and Theorem 2 reduces to Theorem 1.

The Ritz pairs  $(\mu, u)$  are known to be best suited for approximating the extreme eigenpairs of  $A$ , i.e., those  $(\lambda, x)$  that correspond to  $\lambda$  near the boundary of  $A$ 's spectrum, further denoted by  $\Lambda(A)$ . If interior eigenpairs are wanted, then the Rayleigh–Ritz procedure may not be appropriate; it can produce “spurious” or “ghost” Ritz values [7, 13,15].

This problem, however, can be fixed by the use of the *harmonic* Rayleigh–Ritz procedure [7,8,15]. Given a shift  $\sigma$  pointing to a location inside  $\Lambda(A)$ , the harmonic Rayleigh–Ritz scheme aims at finding the harmonic Ritz pairs  $(\theta, v)$  that approximate the eigenpairs  $(\lambda, x)$  of  $A$  associated with the eigenvalues  $\lambda$  closest to  $\sigma$ . This is fulfilled by imposing the Petrov–Galerkin condition

$$Av - \theta v \perp (A - \sigma I)\mathcal{K}, \quad v \in \mathcal{K}, \tag{8}$$

which, similar to (1), gives an  $s$ -by- $s$  eigenvalue problem. In particular, if  $A$  is Hermitian, this eigenvalue problem is of the form

$$K^*(A - \sigma I)^2Kc = \xi K^*(A - \sigma I)Kc. \tag{9}$$

The eigenpairs  $(\xi, c)$  of (9) yield the harmonic Ritz pairs  $(\theta, v)$ , where  $\theta = \xi + \sigma$  is a harmonic Ritz value and  $v = Kc$  is the corresponding harmonic Ritz vector.

In this paper, we present a Saad’s type bound for harmonic Ritz vectors of a Hermitian matrix  $A$ . It shows that, along with  $\angle(x, \mathcal{K})$ , the closeness of the harmonic Ritz vectors to the exact eigenvectors generally depends on the spectral condition number of  $A - \sigma I$ . This property of the harmonic Rayleigh–Ritz procedure is fundamentally different from the standard Rayleigh–Ritz which, according to Theorem 1, is not affected by conditioning of the (shifted) operator.

Our finding has a practical implication. Namely, difficulties related to a poor conditioning of algebraic systems are commonly mitigated by the use of preconditioners; e.g., [4,10]. Therefore, motivated by the dependence on the condition number, one can expect to improve the harmonic Rayleigh–Ritz approximations by properly preconditioning the procedure.

A possible way to blend preconditioning directly into the harmonic Rayleigh–Ritz scheme was proposed in [19]. There, the authors introduce the *T-harmonic* Rayleigh–Ritz procedure, which is defined by the Petrov–Galerkin condition (8) with respect to the inner product  $(\cdot, \cdot)_T = (\cdot, T \cdot)$ , where  $T$  is a Hermitian positive definite (HPD) preconditioner. Within this framework, the eigenpairs of  $A$  are approximated by the *T-harmonic* Ritz pairs  $(\theta, v)$ , such that

$$Av - \theta v \perp_T (A - \sigma I)\mathcal{K}, \quad v \in \mathcal{K}, \quad (10)$$

where  $\perp_T$  denotes orthogonality in the  $T$ -inner product. If  $A$  is Hermitian, the procedure amounts to solving an  $s$ -by- $s$  eigenvalue problem

$$K^*(A - \sigma I)T(A - \sigma I)Kc = \xi K^*(A - \sigma I)TKc. \quad (11)$$

The *T-harmonic* Ritz values are then given by  $\theta = \xi + \sigma$ , whereas the *T-harmonic* Ritz vectors are defined by  $v = Kc$ .

In the present work, we address an idealized situation where the HPD preconditioner  $T$  commutes with  $A$ . In this case, our generalization of the Saad’s bound can further be easily extended to the *T-harmonic* Rayleigh–Ritz. We show that, along with  $\angle(x, \mathcal{K})$ , the proximity of the *T-harmonic* Ritz vectors to the exact eigenvectors depends on the condition number of the matrix  $T^{1/2}(A - \sigma I)$ . In particular, this means that the approximation quality can be improved in practice by properly choosing a preconditioner  $T$ . We briefly discuss several possibilities for defining  $T$ , including the absolute value preconditioning [18,20].

Finally, we note that other generalizations of the Saad’s bound on the harmonic Ritz vectors were obtained in [2,5]. These results, however, aim at general matrices  $A$  and as a consequence do not capture certain peculiarities of the Hermitian case. In particular, the bounds in [2,5] do not reveal the dependence on the condition number. Furthermore, they fail to imply that the harmonic Ritz vectors necessarily converge to the exact eigenvectors as  $\angle(x, \mathcal{K})$  decreases.

The paper is organized as following. Section 2 presents our main result. Related work, such as [2,5], is discussed in Section 3. Section 4 provides an extension of the main theorem on eigenspaces associated with multiple eigenvalues. In Section 5, we consider the case of the *T-harmonic* Rayleigh–Ritz and derive the Saad’s bound for commuting  $A$  and  $T$ . Throughout, we assume that  $A$  is Hermitian.

## 2. A bound for harmonic Ritz vectors

We start with a lemma that provides a two-sided bound on the angle between an eigenvector  $x$  and an arbitrary vector  $y$  in terms of  $\angle(x, Ay)$ . This bound will be crucial for deriving our main result.

**Lemma 1.** *Let  $(\lambda, x)$  be an eigenpair of a nonsingular Hermitian matrix  $A$ . Then for any vector  $y$ , we have*

$$|\lambda/\lambda_{\max}| \sin \angle(x, Ay) \leq \sin \angle(x, y) \leq |\lambda/\lambda_{\min}| \sin \angle(x, Ay), \tag{12}$$

where  $\lambda_{\min}$  and  $\lambda_{\max}$  are the smallest and largest magnitude eigenvalues of  $A$ , respectively.

**Proof.** Let us first introduce the notation  $\phi = \angle(x, y)$ ,  $\phi_A = \angle(x, Ay)$  and observe that  $\phi_A = 0$  if and only if  $\phi = 0$ . Hence, if  $\phi = 0$  then bound (12) is trivial. Therefore, in what follows, we consider only the case where  $0 < \phi \leq \pi/2$ .

Without loss of generality, we assume that both  $x$  and  $y$  are unit vectors. Then, since  $x$  is an eigenvector, we observe that

$$\cos \phi = |x^*y| = \left| \frac{x^*Ay}{\lambda} \right| = \left( \frac{\|Ay\|}{|\lambda|} \right) \left( \frac{|x^*Ay|}{\|Ay\|} \right) = \left( \frac{\|Ay\|}{|\lambda|} \right) \cos \phi_A,$$

where  $\cos \phi = |x^*y|$  and  $\cos \phi_A = |x^*Ay|/\|Ay\|$ . This relation implies that

$$\frac{\sin^2 \phi}{\sin^2 \phi_A} = \frac{\sin^2 \phi}{1 - \cos^2 \phi_A} = \frac{\|Ay\|^2 \sin^2 \phi}{\|Ay\|^2 - \lambda^2 \cos^2 \phi}. \tag{13}$$

Let  $y = x(x^*y) + w(w^*y)$  be a representation of  $y$  in terms of the eigenvector  $x$  and a unit vector  $w$  orthogonal to  $x$ . Then  $\|Ay\|^2 = \lambda^2 \cos^2 \phi + (w^*A^2w) \sin^2 \phi$ , where  $\sin^2 \phi = |w^*y|^2 = \cos^2 \angle(w, y)$ . Substituting this expression into the right-hand side of (13) gives

$$\frac{\sin^2 \phi}{\sin^2 \phi_A} = \left( \frac{\lambda^2}{w^*A^2w} \right) \cos^2 \phi + \sin^2 \phi. \tag{14}$$

By the Courant–Fischer theorem [9,11],  $a_0^2 \leq \lambda^2/(w^*A^2w) \leq a_1^2$ , where

$$a_0^2 = \min_{\substack{q \in x^\perp \\ \|q\|=1}} \frac{\lambda^2}{q^*A^2q} = \frac{\lambda^2}{\max_{\lambda_j \in \Lambda(A) \setminus \lambda} \lambda_j^2}, \tag{15}$$

and

$$a_1^2 = \max_{\substack{q \in x^\perp, \\ \|q\|=1}} \frac{\lambda^2}{q^* A^2 q} = \frac{\lambda^2}{\min_{\lambda_j \in \Lambda(A) \setminus \lambda} \lambda_j^2}. \tag{16}$$

Thus, from (14)–(16), we obtain

$$a_0^2 \cos^2 \phi + \sin^2 \phi \leq \frac{\sin^2 \phi}{\sin^2 \phi_A} \leq a_1^2 \cos^2 \phi + \sin^2 \phi. \tag{17}$$

Let us now consider the function  $f(z; a) = a^2 \cos^2 z + \sin^2 z$ , where  $z$  is a variable and  $a^2$  is a fixed positive parameter. Then (17) can be written as

$$f(\phi; a_0^2) \leq \frac{\sin^2 \phi}{\sin^2 \phi_A} \leq f(\phi; a_1^2). \tag{18}$$

Hence, for any  $0 < \phi \leq \pi/2$ ,

$$\min_{z \in [0, \pi/2]} f(z; a_0^2) \leq \frac{\sin^2 \phi}{\sin^2 \phi_A} \leq \max_{z \in [0, \pi/2]} f(z; a_1^2). \tag{19}$$

It is easy to check, by differentiation, that  $f(z; a^2)$  is monotonically increasing on  $[0, \pi/2]$  if  $a^2 \leq 1$ . If  $a^2 \geq 1$ , then the function is decreasing.

From (15), we see that  $a_0^2 < 1$  if  $\lambda \neq \lambda_{\max}$ , where  $\lambda_{\max}$  is an eigenvalue of  $A$  of the largest absolute value. Therefore, in this case,  $f(z; a_0^2)$  is increasing on  $[0, \pi/2]$  and its minimum is given by  $f(0; a_0^2) = \lambda^2/\lambda_{\max}^2$ . At the same time, if  $\lambda = \lambda_{\max}$ , then  $a_0^2 \geq 1$ , and, hence,  $f(z; a_0^2)$  is decreasing on  $[0, \pi/2]$ . Therefore, the minimum is delivered by  $f(\pi/2; a_0^2) = 1$ . Thus, we get

$$\min_{z \in [0, \pi/2]} f(z; a_0^2) = \begin{cases} \lambda^2/\lambda_{\max}^2, & \text{if } \lambda \neq \lambda_{\max}, \\ 1, & \text{if } \lambda = \lambda_{\max}. \end{cases} \tag{20}$$

After combining the both cases in (20), we conclude that

$$\min_{z \in [0, \pi/2]} f(z; a_0^2) = \lambda^2/\lambda_{\max}^2. \tag{21}$$

Similarly, by (16),  $a_1^2 > 1$  if  $\lambda \neq \lambda_{\min}$ , where  $\lambda_{\min}$  denotes an eigenvalue of  $A$  of the smallest absolute value; and  $a_1^2 \leq 1$  otherwise. By applying exactly the same argument, based on the monotonicity of  $f(z; a_1^2)$ , as above, we obtain

$$\max_{z \in [0, \pi/2]} f(z; a_1^2) = \lambda^2/\lambda_{\min}^2. \tag{22}$$

Substituting (21) and (22) into (19) and taking the square root of all parts of the inequality gives (12).  $\square$

Note that Lemma 1 suggests that, in particular, if  $(\lambda, x)$  is an eigenpair corresponding to the smallest magnitude eigenvalue, then  $\angle(x, y) \leq \angle(x, Ay)$ , i.e., the approximation quality of a vector  $y$  does not improve after multiplication with  $A$ . On the other hand, if  $(\lambda, x)$  is associated with the largest magnitude eigenvalue, then  $\angle(x, y) \geq \angle(x, Ay)$ . The latter is not surprising, because a step of the power method applied to  $y$  is expected to yield a better approximation to the dominant eigenvector.

Given a subspace  $\mathcal{K}$ , the following corollary relates  $\angle(x, \mathcal{K})$  and  $\angle(x, A\mathcal{K})$ .

**Corollary 1.** *Let  $(\lambda, x)$  be an eigenpair of a nonsingular Hermitian matrix  $A$ . Then for any subspace  $\mathcal{K}$  of  $\mathbb{C}^n$ , we have*

$$\sin \angle(x, A\mathcal{K}) \leq |\lambda_{\max}/\lambda| \sin \angle(x, \mathcal{K}). \tag{23}$$

**Proof.** From the left-hand side of (12), we have

$$\sin \angle(x, Ay) \leq |\lambda_{\max}/\lambda| \sin \angle(x, y).$$

This inequality holds for any vector  $y$ . In particular, it is true for some  $y_* \in \mathcal{K}$  that yields the minimum of  $\angle(x, y)$  over all  $y$  in  $\mathcal{K}$ . By definition (2),  $\angle(x, y_*)$  is exactly the angle between the vector  $x$  and the subspace  $\mathcal{K}$ . Thus, we obtain

$$\sin \angle(x, Ay_*) \leq |\lambda_{\max}/\lambda| \sin \angle(x, \mathcal{K}). \tag{24}$$

On the other hand,

$$\angle(x, A\mathcal{K}) = \min_{y \in \mathcal{K}, y \neq 0} \angle(x, Ay) \leq \angle(x, Ay_*).$$

Therefore,  $\sin \angle(x, A\mathcal{K}) \leq \sin \angle(x, Ay_*)$ . Combining this inequality with (24) leads to (23), which completes the proof.  $\square$

We are now ready to state the main result.

**Theorem 3.** *Let  $(\lambda, x)$  be an eigenpair of a Hermitian matrix  $A$  and  $(\theta, v)$  be a harmonic Ritz pair with respect to the subspace  $\mathcal{K}$  and shift  $\sigma \notin \Lambda(A)$ . Assume that  $\Theta$  is a set of all the harmonic Ritz values and let  $P_{\mathcal{Q}}$  be an orthogonal projector onto  $\mathcal{Q} = (A - \sigma I)\mathcal{K}$ . Then*

$$\sin \angle(x, v) \leq \kappa(A - \sigma I) \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{K}), \tag{25}$$

where  $\gamma = \|P_{\mathcal{Q}}(A - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|$ ,

$$\kappa(A - \sigma I) = \frac{\max_{\lambda_j \in \Lambda(A)} |\lambda_j - \sigma|}{\min_{\lambda_j \in \Lambda(A)} |\lambda_j - \sigma|}, \tag{26}$$

and

$$\delta = \min_{\theta_j \in \Theta \setminus \theta} \left| \frac{\theta_j - \lambda}{(\lambda - \sigma)(\theta_j - \sigma)} \right|. \tag{27}$$

**Proof.** We first observe that the eigenvalue problem (9) can be formulated as

$$(SK)^* S^{-1} (SK)c = \tau(SK)^* (SK)c, \quad S = A - \sigma I, \tag{28}$$

where the matrix  $S$  is nonsingular because  $\sigma \notin \Lambda(A)$ . Each eigenpair  $(\tau, c)$  of (28) yields an eigenpair  $(\xi, c)$  of (9) with  $\xi = 1/\tau$ . Thus, given  $(\tau, c)$ , the corresponding harmonic Ritz pair  $(\theta, v)$  is defined by  $\theta = 1/\tau + \sigma$  and  $v = Kc$ .

At the same time, problem (28) corresponds to the Rayleigh–Ritz procedure for the matrix  $S^{-1}$  with respect to the subspace  $\mathcal{Q} = SK$ , in which case a Ritz pair is given by  $(\tau, Sv)$ , where  $v = Kc$  is the harmonic Ritz vector. The eigenvalues of  $S^{-1}$  are related to the eigenvalues  $\lambda$  of  $A$  as  $1/(\lambda - \sigma)$ , and the corresponding eigenvectors  $x$  coincide. Then Theorem 1 guarantees that for an eigenpair  $(1/(\lambda - \sigma), x)$  of  $S^{-1}$  and a Ritz pair  $(\tau, Sv)$ ,

$$\sin \angle(x, Sv) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{Q}), \tag{29}$$

with  $\gamma = \|P_{\mathcal{Q}} S^{-1} (I - P_{\mathcal{Q}})\|$  and, since  $\tau = 1/(\theta - \sigma)$ ,

$$\delta = \min_{\theta_j \in \Theta \setminus \theta} \left| \frac{1}{\lambda - \sigma} - \frac{1}{\theta_j - \sigma} \right| = \min_{\theta_j \in \Theta \setminus \theta} \left| \frac{\theta_j - \lambda}{(\lambda - \sigma)(\theta_j - \sigma)} \right|.$$

Clearly, if  $(\lambda, x)$  is an eigenpair of  $A$  then  $(\lambda - \sigma, x)$  is an eigenpair of  $S$ . Therefore, recalling that  $\mathcal{Q} = SK$ , we can apply Corollary 1 with respect to  $S$  to bound  $\sin \angle(x, \mathcal{Q})$  in (29) from above by a term proportional to  $\sin \angle(x, \mathcal{K})$ . As a result, from (29), we get

$$\sin \angle(x, Sv) \leq \frac{\max_{\lambda_j \in \Lambda(A)} |\lambda_j - \sigma|}{|\lambda - \sigma|} \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{K}). \tag{30}$$

On the other hand, by Lemma 1, also applied with respect to  $S$ , we obtain

$$\sin \angle(x, v) \leq \frac{|\lambda - \sigma|}{\min_{\lambda_j \in \Lambda(A)} |\lambda_j - \sigma|} \sin \angle(x, Sv). \tag{31}$$

The desired bound (25) then follows from (30) and (31).  $\square$

Theorem 3 shows that the approximation quality of the harmonic Rayleigh–Ritz procedure can be hindered by a poor conditioning of  $A - \sigma I$ . In particular, this can happen if the shift  $\sigma$  is chosen to be close to an eigenvalue of  $A$ .



Furthermore, the structure of the quantity  $\delta$  in (27) suggests that the proximity of the harmonic Ritz vectors to exact eigenvectors can be affected by clustering of  $A$ 's eigenvalues, in which case  $\delta$  can be close to zero. The smallness of  $\delta$  can also be caused by a large difference  $|\lambda - \sigma|$  in the denominator of (27). This indicates that the harmonic Rayleigh–Ritz scheme should be most efficient for approximating the eigenpairs associated with the eigenvalues closest to a given shift  $\sigma$ . Note that  $\delta$  is finite, as  $\sigma \neq \lambda$  and  $\theta_j \neq \sigma$  [8, Theorem 2.2].

Bound (25) implies that a harmonic Ritz vector  $v$  must approach the exact eigenvector  $x$  as the angle between  $x$  and the subspace  $\mathcal{K}$  decreases, provided that there is only one harmonic Ritz value that converges to the targeted eigenvalue  $\lambda$ . In the opposite case, which can occur if  $\lambda$  is a multiple eigenvalue, the quantity  $\delta$  converges to zero (the set  $\Theta$  in (27) assumes repetition of multiple harmonic Ritz values). Hence, in this setting, bound (25) may not guarantee that  $\angle(x, v)$  is small whenever  $\angle(x, \mathcal{K})$  is sufficiently small. This limitation, however, is natural as it reflects the fact that the direction of  $x$  is not unique in the case of a multiple  $\lambda$  and that the harmonic Ritz vector can tend to approximate any other element of the associated eigenspace. A proper extension of Theorem 3, which gives a meaningful bound in the case where  $\lambda$  has multiplicity greater than 1, will be considered below in Section 4.

The result of Theorem 3 is very general in that it holds for any choice of the subspace  $\mathcal{K}$ . Hence, it is rather pessimistic. In particular, practical eigensolvers construct the subspace  $\mathcal{K}$ , often called the trial or search subspace, very carefully, in such a way that it does not contain contributions from unwanted eigenvectors.

We address this practical setting in the following corollary. It shows that if  $\mathcal{K}$  is chosen from an invariant subspace of  $A$  associated with only a part of its spectrum, which however contains the wanted eigenvalues, then the condition number in the right-hand side of (25) can be reduced.

**Corollary 2.** *Let  $X$  be a matrix whose columns represent an orthonormal basis of an invariant subspace of  $A$  associated with a subset  $\Lambda_X(A) \subseteq \Lambda(A)$  of its eigenvalues, and assume that  $\mathcal{K} \subseteq \text{range}(X)$ . Let  $(\lambda, x)$  be an eigenpair of  $A$ , such that  $\lambda \in \Lambda_X(A)$ , and let  $(\theta, v)$  be a harmonic Ritz pair with respect to  $\mathcal{K}$  and  $\sigma \notin \Lambda_X(A)$ . Assume that  $\Theta$  is a set of all the harmonic Ritz values and let  $P_{\mathcal{Q}}$  be an orthogonal projector onto  $\mathcal{Q} = X^*(A - \sigma I)\mathcal{K}$ . Then*

$$\sin \angle(x, v) \leq \kappa(X^*AX - \sigma I) \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{K}), \tag{32}$$

where  $\gamma = \|P_{\mathcal{Q}}(X^*AX - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|$ ,

$$\kappa(X^*AX - \sigma I) = \frac{\max_{\lambda_j \in \Lambda_X(A)} |\lambda_j - \sigma|}{\min_{\lambda_j \in \Lambda_X(A)} |\lambda_j - \sigma|}, \tag{33}$$

and  $\delta$  is defined in (27).

**Proof.** Since  $\mathcal{K} \subseteq \text{range}(X)$ , a basis  $K$  of this subspace can be expressed as  $K = XW$ , where  $W$  is a  $k$ -by- $s$  matrix, with  $k$  being the number of columns in  $X$  and  $s = \dim(\mathcal{K})$ . Substituting  $K = XW$  into (9), and using the fact that the columns of  $X$  are orthonormal and span an invariant subspace of  $A$ , gives

$$W^*(X^*AX - \sigma I)^2Wc = \xi W^*(X^*AX - \sigma I)Wc. \tag{34}$$

This eigenvalue problem corresponds to the harmonic Rayleigh–Ritz procedure for the matrix  $X^*AX$  with respect to the subspace  $\mathcal{W} = \text{range}(W) \subseteq \mathbb{C}^k$  and shift  $\sigma$ . The eigenvalues of  $X^*AX$  are exactly the eigenvalues  $\lambda$  of  $A$  in  $\Lambda_X(A)$ , whereas the associated eigenvectors  $\hat{x}$  are related to those of  $A$  by  $x = X\hat{x}$ .

The harmonic Ritz pairs  $(\theta, \hat{v})$  of  $X^*AX$  are defined by the eigenpairs of (34), such that  $\theta = \xi + \sigma$  and  $\hat{v} = Wc$ . Then, by Theorem 3, applied with respect to  $X^*AX$  and  $\mathcal{W}$ , for each eigenpair  $(\lambda, \hat{x})$  of  $X^*AX$  and a harmonic Ritz pair  $(\theta, \hat{v})$ ,

$$\sin \angle(\hat{x}, \hat{v}) \leq \kappa(X^*AX - \sigma I) \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(\hat{x}, \mathcal{W}), \tag{35}$$

where  $\kappa(X^*AX - \sigma I)$  is defined in (33) and  $\gamma = \|P_{\mathcal{Q}}(X^*AX - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|$  with  $\mathcal{Q} = (X^*AX - \sigma I)\mathcal{W} = X^*(A - \sigma I)X\mathcal{W} = X^*(A - \sigma I)\mathcal{K}$ , since  $\mathcal{K} = X\mathcal{W}$ . The quantity  $\delta$  is given by (27), where the set  $\Theta$  of the harmonic Ritz values of  $X^*AX$  with respect to  $\mathcal{W}$  coincides with the harmonic Ritz values of  $A$  over  $\mathcal{K}$ . But  $\angle(\hat{x}, \hat{v}) = \angle(X\hat{x}, X\hat{v}) = \angle(x, v)$ , since  $X$  has orthonormal columns and  $X\hat{v} = XWc = Kc = v$ , where  $v$  is a harmonic Ritz vector of  $A$  with respect to  $\mathcal{K}$  associated with the harmonic Ritz value  $\theta$ . Similarly,  $\angle(\hat{x}, \mathcal{W}) = \angle(X\hat{x}, X\mathcal{W}) = \angle(x, \mathcal{K})$ . Thus, (32) follows from (35).  $\square$

In particular, Corollary 2 implies that choosing  $\mathcal{K}$  from the invariant subspace of  $A$  associated with the eigenvalues  $\{\lambda_1, \lambda_2, \dots, \lambda_k\}$  that are closest to  $\sigma$ , such that  $|\lambda_1 - \sigma| \leq |\lambda_2 - \sigma| \leq \dots \leq |\lambda_k - \sigma|$ , yields the effective condition number of  $|\lambda_k - \sigma|/|\lambda_1 - \sigma|$ , which can be much lower than  $\kappa(A - \sigma I) = |\lambda_n - \sigma|/|\lambda_1 - \sigma|$  suggested by Theorem 3, where  $\lambda_n$  is an eigenvalue of  $A$  that is the most distant from  $\sigma$ . In practice, such a choice of  $\mathcal{K}$  is achieved by damping out the unwanted eigenvector components from a trial subspace, e.g., using filtering or preconditioning techniques; e.g., [3,6,14,17,19].

### 3. Related work

Other bounds for the harmonic Ritz vectors were established in [2,5]. These results are more general than (25) in that they hold for any  $A$ , which can be non-Hermitian. However, as we will see below, in the Hermitian case, which is the focus of this paper, the presented bound (25) turns out to be more descriptive.

In particular, if  $A$  is Hermitian, the result of [2] states that

$$\sin \angle(x, v) \leq \sqrt{1 + \frac{\gamma_1^2 \|B^{-1}\|^2}{\text{sep}(\lambda, G)^2}} \sin \angle(x, \mathcal{K}), \tag{36}$$

where  $B = K^*(A - \sigma I)K$ ,  $\gamma_1 = \|P_{\mathcal{K}}(A - \sigma I)(A - \lambda I)(I - P_{\mathcal{K}})\|$ , and  $P_{\mathcal{K}}$  denotes an orthogonal projector onto  $\mathcal{K}$ . The quantity

$$\text{sep}(\lambda, G) = \|(G - \lambda I)^{-1}\|^{-1}$$

describes separation of the targeted eigenvalue  $\lambda$  from the harmonic Ritz values different from the one associated with  $v$ , which are the eigenvalues of  $G$ ; see [2] for the precise definition of  $G$ .

The result of [5] suggests that

$$\sin \angle(x, v) \leq \left( 1 + \frac{2\|B^{-1}\|^2\gamma_2^2}{\sqrt{1 - \sin^2 \angle(x, \mathcal{K})}\text{sep}(\lambda, G)} \right) \sin \angle(x, \mathcal{K}), \tag{37}$$

where, if  $A$  is Hermitian, the matrix  $B = K^*(A - \sigma I)K$  is the same as in (36) and  $\gamma_2$  is the maximum value of  $|\lambda - \sigma|$  over all eigenvalues  $\lambda$  of  $A$ . Similarly,  $\text{sep}(\lambda, G)$  gives a separation of  $\lambda$  from the unwanted harmonic Ritz values.

Both (36) and (37) share a number of similarities with the bound (25) of this paper. In particular, all of them show that the approximation quality of a Ritz vector depends on  $\angle(x, \mathcal{K})$ , separation of  $\lambda$ , and the choice of the shift  $\sigma$ , which should not be too close to an eigenvalue.

However, the main difference of (25) is that it eliminates the dependence of the bound on the norm of  $B^{-1} = (K^*(A - \sigma I)K)^{-1}$ . This norm can generally be large or unbounded, even if  $\sigma$  is well chosen, the subspace  $\mathcal{K}$  contains a good eigenvector approximation, and the corresponding eigenvalue is well separated. As a result, bound (25) guarantees that, if  $\lambda$  is a simple eigenvalue, a harmonic Ritz vector  $v$  must converge to the eigenvector  $x$  as the angle between  $\mathcal{K}$  and  $x$  decreases (the same conclusion for eigenvalues of a higher multiplicity is obtained in the next section). By contrast, neither (36) nor (37) can lead to this conclusion without an additional assumption on the uniform boundedness of  $\|B\|^{-1}$ ; see [2,5].

#### 4. Extension on eigenspaces

As has already been discussed in Section 2, bound (25) is not useful if the targeted eigenvector  $x$  corresponds to an eigenvalue  $\lambda$  of multiplicity greater than 1. In this case, instead of an individual eigenvector  $x$ , the focus should be shifted on the eigenspace  $\mathcal{X}$  associated with  $\lambda$ . In particular, a question to ask is whether there exist a subspace  $\mathcal{V}$  spanned by harmonic Ritz vectors extracted from  $\mathcal{K}$ , which gives a good approximation to  $\mathcal{X}$ , provided that  $\mathcal{K}$  contains a good approximation to the wanted eigenspace  $\mathcal{X}$ .

We note that a similar limitation is also true for the original Saad’s bound of [Theorem 1](#). Fortunately, the Stewart’s [Theorem 2](#) suggests an appropriate extension on eigenspaces, which is stated in the following corollary.

**Corollary 3.** *Let  $\mathcal{X}$  be an eigenspace associated with an eigenvalue  $\lambda$  of  $A$ , and let  $\mathcal{U}$  be a subspace spanned by Ritz vectors associated with Ritz values  $\Theta_k = \{\mu_1, \mu_2, \dots, \mu_k\}$  with respect to  $\mathcal{K}$ . Assume that  $\Theta$  is a set of all the Ritz values and let  $P_{\mathcal{K}}$  be an orthogonal projector onto  $\mathcal{K}$ . Then*

$$\sin \angle(\mathcal{X}, \mathcal{U}) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(\mathcal{X}, \mathcal{K}), \tag{38}$$

where  $\gamma = \|P_{\mathcal{K}}A(I - P_{\mathcal{K}})\|_F$  and  $\delta$  is defined by

$$\delta = \min_{\mu_j \in \Theta \setminus \Theta_k} |\lambda - \mu_j|. \tag{39}$$

**Proof.** We apply [Theorem 2](#) to the subspaces  $\mathcal{X}$  and  $\mathcal{U}$ , such that  $\mathcal{X}$  is an eigenspace of  $\lambda$  and  $\mathcal{U}$  is the Ritz subspace associated with  $\Theta_k$ ; and choose  $\|\cdot\|$  to be the Frobenius norm. This immediately yields bound (38), where  $\gamma = \|P_{\mathcal{K}}A(I - P_{\mathcal{K}})\|_F$ . It then only remains to determine the value of  $\delta$ .

Using the fact that  $\mathcal{X}$  is an eigenspace of  $\lambda$ , from (6), we obtain

$$\delta^2 = \min_{\|Z\|_F=1} \|(V^*AV)Z - Z(X^*AX)\|_F^2 = \min_{\|Z\|_F=1} \|(V^*AV)Z - \lambda Z\|_F^2,$$

where the columns of  $X$  and  $V$  represent orthonormal bases of  $\mathcal{X}$  (i.e.,  $AX = \lambda X$ ) and of the orthogonal complement of  $\mathcal{U}$  in  $\mathcal{K}$ , respectively. If  $m$  is the multiplicity of  $\lambda$  and  $s$  is the dimension of  $\mathcal{K}$ , then  $Z$  is an  $(s - k)$ -by- $m$  matrix. Thus, the above equality can be written as

$$\begin{aligned} \delta^2 &= \min_{\|z_1\|^2 + \dots + \|z_m\|^2 = 1} \sum_{i=1}^m \|(V^*AV - \lambda I)z_i\|^2 \\ &= \min_{\|z_1\|^2 + \dots + \|z_m\|^2 = 1} \sum_{i=1}^m ((V^*AV - \lambda I)^2 z_i, z_i), \end{aligned} \tag{40}$$

where  $z_i$  denote the columns of  $Z$ . By the Courant–Fischer theorem [\[9,11\]](#),

$$((V^*AV - \lambda I)^2 z_i, z_i) \geq \zeta^2 \|z_i\|^2, \quad i = 1, \dots, m;$$

where  $\zeta^2$  is the smallest eigenvalue of  $(V^*AV - \lambda I)^2$ . Therefore,

$$\sum_{i=1}^m ((V^*AV - \lambda I)^2 z_i, z_i) \geq \zeta^2 \sum_{i=1}^m \|z_i\|^2. \tag{41}$$

Taking minimum of both sides of (41) over vectors  $z_i$ , such that  $\sum_{i=1}^m \|z_i\|^2 = 1$ , gives the inequality

$$\min_{\|z_1\|^2 + \dots + \|z_m\|^2 = 1} \sum_{i=1}^m ((V^*AV - \lambda I)^2 z_i, z_i) \geq \zeta^2,$$

which turns into equality if all  $z_i$  are set to an eigenvector associated with the eigenvalue  $\zeta^2$ , normalized to have a norm of  $1/\sqrt{m}$ . Hence,

$$\min_{\|z_1\|^2 + \dots + \|z_m\|^2 = 1} \sum_{i=1}^m ((V^*AV - \lambda I)^2 z_i, z_i) = \zeta^2,$$

and, from (40), we conclude that  $\delta^2 = \zeta^2$ . But the eigenvalues of  $V^*AV$  are the Ritz values with respect to  $\mathcal{K}$  that are different from those in  $\Theta_k$ . Therefore,  $\zeta^2 = \min_{\mu_j \in \Theta \setminus \Theta_k} (\lambda - \mu_j)^2$ , which gives (39), and completes the proof.  $\square$

Note that a similar statement can be obtained from Theorem 2 using the spectral norm in the definition of  $\gamma$  and  $\delta$ . In this case, one arrives at bound (38) with  $\gamma = \|P_{\mathcal{K}}A(I - P_{\mathcal{K}})\|$ , where  $\|\cdot\|$  is the spectral norm. However, the separation constant  $\delta$  will no longer be of the form (39), and instead should be determined according to (6), with  $X^*AX = \lambda I$ , which is somewhat less intuitive. For this reason, we prefer to use the Frobenius norm in Corollary 3.

In order to extend Theorem 3 on eigenspaces, we will need the following result, which is an immediate corollary of Lemma 1.

**Corollary 4.** *Let  $\mathcal{X}$  be an eigenspace associated with an eigenvalue  $\lambda$  of a nonsingular Hermitian matrix  $A$ . Then for any subspace  $\mathcal{Y}$ , we have*

$$|\lambda/\lambda_{\max}| \sin \angle(\mathcal{X}, A\mathcal{Y}) \leq \sin \angle(\mathcal{X}, \mathcal{Y}) \leq |\lambda/\lambda_{\min}| \sin \angle(\mathcal{X}, A\mathcal{Y}), \tag{42}$$

where  $\lambda_{\min}$  and  $\lambda_{\max}$  are the smallest and largest magnitude eigenvalues of  $A$ , respectively.

**Proof.** Let vectors  $x_* \in \mathcal{X}$  and  $y_* \in \mathcal{Y}$  deliver the minimum of  $\angle(x, y)$  for all  $x \in \mathcal{X}$  and  $y \in \mathcal{Y}$ , so that, by definition (7),  $\angle(x_*, y_*) = \angle(\mathcal{X}, \mathcal{Y})$ . Since  $x_*$  is an eigenvector corresponding to  $\lambda$ , we can readily apply inequality (12) of Lemma 1 with  $x = x_*$  and  $y = y_*$ . In particular, the left-hand side of (12) yields the bound

$$|\lambda/\lambda_{\max}| \sin \angle(x_*, Ay_*) \leq \sin \angle(\mathcal{X}, \mathcal{Y}). \tag{43}$$

At the same time, by definition (7),

$$\angle(\mathcal{X}, A\mathcal{Y}) = \min_{\substack{x \in \mathcal{X}, x \neq 0 \\ y \in \mathcal{Y}, y \neq 0}} \angle(x, Ay) \leq \angle(x_*, Ay_*).$$

Therefore, after combining the above inequality with (43), we obtain

$$|\lambda/\lambda_{\max}| \sin \angle(\mathcal{X}, A\mathcal{Y}) \leq |\lambda/\lambda_{\max}| \sin \angle(x_*, Ay_*) \leq \sin \angle(\mathcal{X}, \mathcal{Y}),$$

which proves the left part of (42). The right part,

$$\sin \angle(\mathcal{X}, \mathcal{Y}) \leq |\lambda/\lambda_{\min}| \sin \angle(\mathcal{X}, A\mathcal{Y})$$

is proved analogously by choosing  $x_*$  and  $y_*$  that give the minimum of  $\angle(x, Ay)$  over  $x \in \mathcal{X}$  and  $y \in \mathcal{Y}$  and applying the right-hand side of inequality (12) with  $x = x_*$  and  $y = y_*$ .  $\square$

We now state the main result of this section.

**Theorem 4.** *Let  $\mathcal{X}$  be an eigenspace associated with an eigenvalue  $\lambda$  and let  $\mathcal{V}$  be a subspace spanned by harmonic Ritz vectors associated with harmonic Ritz values  $\Theta_k = \{\theta_1, \theta_2, \dots, \theta_k\}$  with respect to the subspace  $\mathcal{K}$  and shift  $\sigma \notin \Lambda(A)$ . Assume that  $\Theta$  is a set of all the harmonic Ritz values and let  $P_{\mathcal{Q}}$  be an orthogonal projector onto  $\mathcal{Q} = (A - \sigma I)\mathcal{K}$ . Then*

$$\sin \angle(\mathcal{X}, \mathcal{V}) \leq \kappa(A - \sigma I) \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(\mathcal{X}, \mathcal{K}), \tag{44}$$

where  $\gamma = \|P_{\mathcal{Q}}(A - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|_F$ ,  $\kappa(A - \sigma I)$  is the condition number defined in (26), and

$$\delta = \min_{\theta_j \in \Theta \setminus \Theta_k} \left| \frac{\theta_j - \lambda}{(\lambda - \sigma)(\theta_j - \sigma)} \right|. \tag{45}$$

**Proof.** As has been established in the proof of Theorem 3, the harmonic Ritz pairs  $(\theta, v)$  of  $A$  with respect to  $\mathcal{K}$  and  $\sigma$  are related to the Ritz pairs  $(\tau, u)$  of  $(A - \sigma)^{-1}$  over the subspace  $\mathcal{Q}$ , so that  $\theta = 1/\tau + \sigma$  and  $u = (A - \sigma I)v$ . Therefore, if  $\mathcal{V}$  is a subspace spanned by harmonic Ritz vectors associated with harmonic Ritz values in  $\Theta_k$ , then  $\mathcal{U} = (A - \sigma I)\mathcal{V}$  is a Ritz subspace associated with Ritz values  $\{1/(\theta_1 - \sigma), 1/(\theta_2 - \sigma), \dots, 1/(\theta_k - \sigma)\}$  of  $(A - \sigma)^{-1}$ . Then, from Corollary 3, applied to matrix  $(A - \sigma)^{-1}$  and subspace  $\mathcal{Q}$ , we obtain

$$\sin \angle(\mathcal{X}, (A - \sigma I)\mathcal{V}) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(\mathcal{X}, \mathcal{Q}), \tag{46}$$

where  $\gamma = \|P_{\mathcal{Q}}(A - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|_F$  and  $\delta$  is defined in (45). Applying inequalities (42) of Corollary 4 (with  $A$  replaced by  $A - \sigma I$ ) to both sides of (46) leads to the desired bound (44), where  $\kappa(A - \sigma I)$  is defined in (26).  $\square$

**Theorem 4** shows that if  $\lambda$  is a multiple eigenvalue, then there exists a subspace  $\mathcal{V}$  spanned by harmonic Ritz vectors that approximates the entire eigenspace  $\mathcal{X}$  associated with  $\lambda$ . Moreover, the approximation is improved as the angle between  $\mathcal{K}$  and  $\mathcal{X}$  decreases.

**5. A bound for  $T$ -harmonic Ritz vectors**

As demonstrated in [19], the robustness of an interior eigensolver can be notably improved by incorporating a properly chosen HPD preconditioner  $T$  into the harmonic Rayleigh–Ritz. This was done by replacing the Petrov–Galerkin condition (8) by (10), which lead to the  $T$ -harmonic Rayleigh–Ritz procedure.

The next theorem shows that our main result can be easily extended to the  $T$ -harmonic case under the idealized assumption that  $A$  and  $T$  commute.

**Theorem 5.** *Let  $(\lambda, x)$  be an eigenpair of a Hermitian matrix  $A$  and  $(\theta, v)$  be a  $T$ -harmonic Ritz pair with respect to the subspace  $\mathcal{K}$  and shift  $\sigma \notin \Lambda(A)$ . Let  $T$  be an HPD preconditioner, such that  $TA = AT$ . Assume that  $\Theta$  is a set of all the  $T$ -harmonic Ritz values and let  $P_{\mathcal{Q}}$  be an orthogonal projector onto  $\mathcal{Q} = T^{1/2}(A - \sigma I)\mathcal{K}$ . Then*

$$\sin \angle(x, v) \leq \kappa(T^{1/2}(A - \sigma I)) \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{K}), \tag{47}$$

with  $\gamma = \|P_{\mathcal{Q}}(A - \sigma I)^{-1}(I - P_{\mathcal{Q}})\|$ ,  $\delta$  defined in (27), and  $\kappa(T^{1/2}(A - \sigma I)) = |\nu_{\max}/\nu_{\min}|$ , where  $\nu_{\min}$  and  $\nu_{\max}$  are the smallest and largest magnitude eigenvalues of  $T^{1/2}(A - \sigma I)$ , respectively.

**Proof.** If  $A$  and  $T$  commute, then (11) can be written as

$$(T^{1/2}SK)^* S^{-1}(T^{1/2}SK)c = \tau(T^{1/2}SK)^*(T^{1/2}SK)c, \quad S = A - \sigma I. \tag{48}$$

This corresponds to the Rayleigh–Ritz procedure for  $S^{-1}$  with respect to the subspace  $\mathcal{Q} = T^{1/2}SK$ , where  $(\tau, T^{1/2}Sv)$  is a Ritz pair, and  $v = Kc$  is the  $T$ -harmonic Ritz vector. Thus, Theorem 1 applies. It suggests that for an eigenpair  $(1/(\lambda - \sigma), x)$  of  $S^{-1}$  and a Ritz pair  $(\tau, T^{1/2}Sv)$ , we have

$$\sin \angle(x, T^{1/2}Sv) \leq \sqrt{1 + \frac{\gamma^2}{\delta^2}} \sin \angle(x, \mathcal{Q}), \tag{49}$$

with  $\gamma = \|P_{\mathcal{Q}}S^{-1}(I - P_{\mathcal{Q}})\|$  and  $\delta$  defined in (27), where  $\Theta$  is the set of all  $T$ -harmonic Ritz values with respect to  $\mathcal{K}$ , as  $\tau$  is related to  $\theta$  by  $\tau = 1/(\theta - \sigma)$ .

Since  $T$  and  $A$  commute, the matrix  $T^{1/2}S$  is Hermitian and nonsingular, because  $\sigma \notin \Lambda(A)$ . Moreover,  $T^{1/2}S$  has the same eigenvectors  $x$  as  $A$ . Therefore, Lemma 1 can be applied with respect to  $T^{1/2}S$ , which gives

$$\sin \angle(x, v) \leq \left| \frac{\nu}{\nu_{\min}} \right| \sin \angle(x, T^{1/2}Sv), \quad (50)$$

where  $\nu$  is an eigenvalue of  $T^{1/2}S$  associated with the eigenvector  $x$  and  $\nu_{\min}$  is the smallest magnitude eigenvalue of  $T^{1/2}S$ . Similarly, by [Corollary 1](#),

$$\sin \angle(x, \mathcal{Q}) \leq \left| \frac{\nu_{\max}}{\nu} \right| \sin \angle(x, \mathcal{K}). \quad (51)$$

Combining [\(50\)](#) and [\(51\)](#) with [\(49\)](#) gives the desired bound [\(48\)](#).  $\square$

Clearly, the assumption that  $TA = AT$  is impractical in general. Nevertheless, the result of [Theorem 5](#) is useful in that it provides qualitative guidelines on the practical choice of the preconditioner  $T$ . For example, it suggests an insight into ideal choices of  $T$ , discussed below.

A possible option for choosing a commuting HPD preconditioner is  $T = |A - \sigma I|^{-1}$ . In this case,  $\kappa(T^{1/2}(A - \sigma I))$  in [\(47\)](#) turns into  $\kappa(A - \sigma I)^{1/2}$ , i.e., the condition number in bound [\(25\)](#) for the conventional harmonic Rayleigh–Ritz is replaced by its square root.

The construction of the exact inverted absolute value is generally infeasible for large problems. However, in practice, one can choose  $T$  as an approximation to  $|A - \sigma I|^{-1}$ . This strategy is called the absolute value preconditioning [\[18,20\]](#). Absolute value preconditioners have been successfully constructed and applied for computing interior eigenvalues of certain classes of matrices in [\[19\]](#).

Another alternative is to set  $T = (A - \sigma I)^{-2}$ . In this case,  $\kappa(T^{1/2}(A - \sigma I))$  in [\(47\)](#) is annihilated. Thus, in practice, a possible approach is to build  $T$  as an approximation of  $(A - \sigma I)^{-2}$ . This, e.g., relates the construction of  $T$  to preconditioning normal equations; see [\[1,12\]](#) for a few options. Generally, however, it is hard to say which of the two preconditioning options is more efficient in practice; the outcomes are likely to be problem dependent.

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