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ACCURATE APPROXIMATIONS TO EIGENPAIRS USING THE HARMONIC RAYLEIGH-RITZ METHOD

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Abstract. The problem in this paper is to construct accurate approximations from a subspace to eigenpairs for symmetric matrices using the harmonic Rayleigh-Ritz method. Morgan introduced this concept in [14] as an alternative for Rayleigh-Ritz in large scale iterative methods for computing interior eigenpairs. The focus rests on the choice and influence of the shift and error estimation. We also give a discussion of the differences and similarities with the refined Ritz approach for symmetric matrices. Using some numerical experiments we compare different conditions for selecting appropriate harmonic Ritz vectors.

Key words. Rayleigh-Ritz; Harmonic Rayleigh-Ritz; refined Ritz; Lehmann intervals

AMS subject classification. 65F15, 65F50

1 Introduction

In some applications it is necessary to compute a few eigenvectors corresponding to eigenvalues in the interior of the spectrum of a symmetric matrix A. Or for short, find a pair (λ, x) (with $x \neq 0$) that satisfies

$$Ax = \lambda x \ .$$

Iterative methods are often the only option when the matrix A is very large and sparse. Well-known examples of such methods include the Lanczos method [17, Chapter 13], the Davidson method [4] and Jacobi-Davidson [20], to mention only a few. All methods mentioned (implicitly) build up a subspace that contains an approximation for the desired eigenvector and subsequently apply a projection technique to construct an approximate eigenpair from the obtained subspace. The subspace projection is often seen as a way to accelerate the convergence of a simple iteration in a similar fashion as, for example, GMRES can be viewed as an accelerated version of Richardson iteration. However, in the context of eigenvalue methods the situation is often more complicated because an approximate eigenpair from the subspace is frequently used in the computation of a vector to expand the subspace or for restarts. Then the success of such a method crucially depends on the success of the subspace projection in constructing a good eigenvector approximation.

The best known method for obtaining approximations from a subspace is Rayleigh-Ritz. This method is optimal for exterior eigenvalues, see for example Section 11.4 in [17]. However, when searching for eigenvectors with eigenvalues in the interior of the spectrum, the situation can be less favorable [18, 9, 14].

There are various efforts to overcome this problem. For example, Scott [18] discusses that working with a shifted and inverted operator in the Rayleigh-Ritz method is preferable. Morgan recognized and proposed in [14] that the required inversion of the operator can be

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handled implicitly with a particular choice for the subspace. The resulting method has been given the name *harmonic* Rayleigh-Ritz in [16]. The eigenvalue approximations corresponding to this method (harmonic Ritz values) have received considerable attention due to their connection with the polynomials of iterative minimal residual methods for linear systems (Kernel polynomials), see [5, 13, 16] for some recent work, and have also been studied in the context of Lehmann's optimal intervals [11, 12, 17, 1].

In this paper we discuss some observations on the harmonic Rayleigh-Ritz method when used to compute approximate eigenpairs for symmetric matrices. The paper is organized as follows. In Section 2 we give a definition of harmonic Rayleigh-Ritz and in Section 3 some useful properties are summarized. The question of which shift results in the best eigenvector approximation is treated in Section 4. This is done by exploiting a relation between *refined* Ritz vectors [8] and the harmonic Ritz vectors. Section 5 contains a discussion on a priori error bounds for the harmonic Ritz pairs.

By changing the shift in the harmonic Rayleigh-Ritz method different intervals can be obtained that at least contain one eigenvalue. In Section 6 we give a condition for a posteriori choosing a new shift that results in a smaller inclusion interval. Applying this condition repeatedly will ultimately result in an, evidently appealing, optimal interval with respect to the given information. Some more specific relations between the harmonic Ritz pairs and Ritz pairs for Krylov subspaces is given in Section 7. Finally, Section 8 illustrates a few numerical experiments with different conditions for the selection of an appropriate harmonic Ritz vector.

2 Harmonic Rayleigh-Ritz

The matrix A is n by n and symmetric and we assume that the eigenpairs of which the eigenvalue is close to some shift σ are of importance. The eigenpairs (λ_j, x_j) of A are numbered such that

$$\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n.$$

Let $V \in \mathbb{R}^{k\times n}$ be an orthonormal matrix, whose columns span the k dimensional subspace $\mathcal{V}$. We are interested in techniques that compute approximations to (interior) eigenpairs, only using information about $\mathcal{V}$ and $A\mathcal{V}$. The most important method in this class is *Rayleigh-Ritz*.

The Rayleigh-Ritz approach gives k approximate eigenpairs (θ_i, u_i), the so-called Ritz pairs, by imposing the Ritz-Galerkin condition

$$Au_i - \theta_i u_i \perp \mathcal{V} \text{ with } u_i \in \mathcal{V}\backslash\{0\},$$

or equivalently,

$$V^T A V z_i - \theta_i z_i = 0 \text{ with } u_i \equiv V z_i \neq 0\ . \tag{1}$$

The vector u_i is called a Ritz vector, the corresponding eigenvalue approximation (Ritz value) can be computed from the Ritz vector by using the Rayleigh quotient

$$\theta_i = \rho(u_i) \text{ where } \rho(v) \equiv \frac{v^T A v}{v^T v}.$$

From (1) it easily follows that the Ritz values are real. We assume that they are ordered and $\|u_i\|_2 = 1$.

It is well-known that Rayleigh-Ritz is not optimal for eigenpairs with eigenvalues in the interior of the spectrum, see [18], [17, Section 11.6], [9]. The problem is that the eigenvectors of the projected system (V^TAV) can be ill-conditioned if two Ritz values are close. This can cause that there are no Ritz vectors offering a good approximation to the eigenvector x, even if $\mathcal{V}$ makes a small angle with x. Due to the Interlace property of the Ritz values (Theorem 10.1.1 in [17]) we know that there cannot be two Ritz values arbitrary close to λ_1 (or for that matter λ_n) and, therefore, the Rayleigh-Ritz method is robust for eigenvalues in the exterior of the spectrum.

A simple strategy to make Rayleigh-Ritz work for interior eigenpairs is to apply it to $(A-\tau I)^2$ if the interesting eigenvalues are close to τ, e.g. [14]. This gives

$$(A-\tau I)^2\widehat{u}_i - \widehat{\theta}_i\widehat{u}_i \perp \mathcal{V} \text{ with } \widehat{u}_i \in \mathcal{V}\backslash\{0\},$$

or,

$$V^T(A-\tau I)^2V\widehat{z}_i - \widehat{\theta}_i\widehat{z}_i = 0 \text{ with } u_i \equiv V\widehat{z}_i \neq 0\ . \tag{2}$$

A potential problem with this approach is that squaring a matrix with a shift close to an eigenvalue in general squares the condition number of the eigenvector (see [2, Section 2.3] for a definition). This can result in loss of precision. Applying Rayleigh-Ritz on $(A-\sigma I)^{-1}$ is then preferable. Morgan [14] proposed to use a subspace $(A-\sigma I)\mathcal{V}$ to circumvent the explicit inversion of the matrix A, which results in *harmonic Rayleigh-Ritz*. We use the following equivalent definition [20, Theorem 5.1] which does not require the existence of the inverse of A. The harmonic Ritz pairs $(\widetilde{\theta}_i, \widetilde{u}_i)$ w.r.t. a shift σ are given by imposing the Petrov-Galerkin condition

$$(A-\widetilde{\theta}_iI)\widetilde{u}_i \perp (A-\sigma I)\mathcal{V} \text{ with } \widetilde{u}_i \in \mathcal{V}\backslash\{0\},$$

or as generalized eigenvalue problem,

$$V^T(A-\sigma I)^2V\widetilde{z}_i - (\widetilde{\theta}_i-\sigma)V^T(A-\sigma I)V\widetilde{z}_i = 0 \text{ with } \widetilde{u}_i \equiv V\widetilde{z}_i \neq 0\ . \tag{3}$$

The harmonic Ritz values $(\widetilde{\theta}_i)$ can be computed from the harmonic Ritz vectors $\widetilde{u}_i$ by using the *harmonic Rayleigh-quotient* (sometimes referred to as Temple quotient [3, Equation (8.31)])

$$\widetilde{\theta}_i = \widetilde{\rho}_\sigma(\widetilde{u}_i) \text{ where } \widetilde{\rho}_\sigma(v) \equiv \sigma + \frac{v^T(A-\sigma I)^2v}{v^T(A-\sigma I)v}. \tag{4}$$

In principle it can happen that $\widetilde{u}^T(A-\sigma I)\widetilde{u} = 0$ in (4), in this case we will write $\widetilde{\theta} = \infty$. Furthermore, we index the harmonic Ritz values as follows

$$\widetilde{\theta}_{-l} \leq \ldots \leq \widetilde{\theta}_{-1} < \sigma < \widetilde{\theta}_1 \leq \ldots \leq \widetilde{\theta}_{k-l}.$$

Whereas the harmonic Ritz approach is related to Rayleigh-Ritz on $(A-\sigma I)^{-1}$, naively we would expect that choosing σ equal to the eigenvalue of interest results in an optimal eigenvector approximation. It turns out, however, that due to the special structure of the test- and search-space this is not necessary optimal. Two of the questions we address in this paper are the influence of the shift σ on the quality of the harmonic Ritz vector and if this method offers advantages over (2), see Section 4.

3 Some useful properties

We summarize some properties of the harmonic Rayleigh-Ritz method that turn out to be useful in the rest of this paper. For simplicity it is assumed, without loss of generality, that $\sigma = 0$.

Lemma 3.1. *Let AV have full rank, $\sigma = 0$, $\dim(\mathcal{V}) = k$ and let there be l negative Ritz values and let zero be a Ritz value with multiplicity m (≥ 0).*
Then there exist k real reciprocals of harmonic Ritz values $\widetilde{\theta}_i^{-1}$, of which l are negative and m are zero. To match them there are k linear independent $\widetilde{u}_i$.
Moreover,

$$\widetilde{u}_i^T A \widetilde{u}_j = 0, \quad \widetilde{u}_i^T A^2 \widetilde{u}_j = 0, \quad \text{if } i \neq j.$$

Proof. The matrix $V^T A^2 V$ is symmetric. Since it also has full rank it is positive definite and the Cholesky decomposition $LL^T = V^T A^2 V$ exists. Then $\widetilde{z}_i = L^T y_i$ with $(\widetilde{\theta}_i^{-1}, y_i)$ an eigenpair of $B = L^{-1} V^T A V L^{-T}$. The $\widetilde{\theta}_i^{-1}$ are real, possibly zero, because of the symmetry of this operator. Sylvester's law of inertia (Fact 1.6 in [17]) shows that the number of positive, negative and zero eigenvalues of $V^T A V$ equals these numbers for B. Finally, the A- and A^2-orthogonality follow easily from the orthogonality and B-orthogonality of the y_i. $\square$

This lemma shows that the number of zero Ritz values equals the number of reciprocals of harmonic Ritz values that are zero (remember that we write $\widetilde{\theta} = \infty$ in this case).

A useful characterization of the harmonic Ritz values is the following formulation of the minmax property, see also [11, Satz 5]

Lemma 3.2. *Let AV have full rank, $\dim(\mathcal{V}) = k$, $\sigma = 0$ and let there be l negative Ritz values and let zero be a Ritz value with multiplicity m. In this case*

$$\frac{1}{\widetilde{\theta}_j} = \max_{\mathcal{S} \subset \mathcal{V}, \dim(\mathcal{S}) = j} \ \min_{u \in \mathcal{S}, u \neq 0} \frac{u^T A u}{u^T A^2 u} \quad j \in \{1, \ldots, k - l - m\}$$

$$\frac{1}{\widetilde{\theta}_{-j}} = \min_{\mathcal{S} \subset \mathcal{V}, \dim(\mathcal{S}) = j} \ \max_{u \in \mathcal{S}, u \neq 0} \frac{u^T A u}{u^T A^2 u} \quad j \in \{1, \ldots, l\}.$$

Proof. Using the matrix B defined in the proof of Lemma 3.1, the minmax characterization (Theorem 10.2.1 in [17]) yields for $j > 1$

$$\frac{1}{\widetilde{\theta}_j} = \max_{\mathcal{S} \subset \mathbb{R}^k, \dim(\mathcal{S}) = j} \ \min_{y \in \mathcal{S}, y \neq 0} \frac{y^T B y}{y^T y} = \max_{\mathcal{S} \subset \mathbb{R}^k, \dim(\mathcal{S}) = j} \ \min_{\widetilde{z} \in \mathcal{S}, \widetilde{z} \neq 0} \frac{\widetilde{z}^T V^T A V \widetilde{z}}{\widetilde{z}^T V^T A^2 V \widetilde{z}}$$

$$= \max_{\mathcal{S} \subset \mathcal{V}, \dim(\mathcal{S}) = j} \ \min_{\widetilde{u} \in \mathcal{S}, \widetilde{u} \neq 0} \frac{\widetilde{u}^T A \widetilde{u}}{\widetilde{u}^T A^2 \widetilde{u}}.$$

A similar argument can be used for the negative harmonic Ritz values. $\square$

The following lemma is an application of the minmax property.

Lemma 3.3. *Let AV have full rank, $\sigma = 0$ and let there be l negative and $k - l$ positive Ritz values. Then*

$$0 < \theta_{l+j} \leq \widetilde{\theta}_j \quad j \in \{1, \ldots, k - l\}$$

$$0 > \theta_{l+1-j} \geq \widetilde{\theta}_{-j} \quad j \in \{1, \ldots, l\}.$$

Proof. We proof the first statement. With $T \equiv V^T AV$ and $R \equiv AV - VT$ we have that $AV = VT + R$ and $V^T R = 0$. Hence, $V^T A^2 V = T^2 + R^T R \geq T^2$. We know from Lemma 3.1 that θ_{l+j} and $\widetilde{\theta}_j$ for $j \geq 1$ are positive. Since $Tz_i = \theta_i z_i$, $Tz_i = \theta_i^{-1} T^2 z_i$ and using the minmax property for generalized eigenvalue problems gives

$$\frac{1}{\theta_{l+j}} = \max_{\mathcal{S} \subset \mathbb{R}^k, \dim(\mathcal{S})=j} \min_{y \in \mathcal{S}, y \neq 0} \frac{y^T T y}{y^T T^2 y}$$

$$\geq \max_{\mathcal{S} \subset \mathbb{R}^k, \dim(\mathcal{S})=j} \min_{y \in \mathcal{S}, y \neq 0} \frac{y^T T y}{y^T (T^2 + R^T R) y} = \frac{1}{\widetilde{\theta}_j}.$$

□

The last lemma can be seen as a variant of Theorem 2.1 from [1] for positive definite matrices. It shows that there are no harmonic Ritz values closer to the origin than a Ritz value.

Just like the Ritz values, the harmonic Ritz values provide information about the eigenvalues that is optimal in some sense. Paige, Parlett and Van der Vorst [16] pointed out an important relation between Lehmann intervals and harmonic Rayleigh-Ritz. They showed that the harmonic Ritz values with respect to the shift σ give Lehmann's optimal intervals.

Proposition 3.1 (Lehmann [11, Satz 9]). *Let σ be any number.*
Each interval $[\widetilde{\theta}_{-i}, \sigma]$, $i = 1, \ldots, l$ contains at least i eigenvalues of A. Each interval $[\sigma, \widetilde{\theta}_i]$, $i = 1, \ldots, k-l$, contains at least i of A's eigenvalues. Moreover there exists an A with only eigenvalues at the end points of all these intervals.

This shows that the harmonic Ritz values provide outer bounds for the eigenvalues. Another consequence is that if $\lambda_{p-1} < \sigma < \lambda_p < \lambda_{p+1}$ there can at most be one harmonic Ritz value in the interval $[\lambda_p, \lambda_{p+1})$ and no $\widetilde{\theta}$ such that $0 \leq \widetilde{\theta} < \lambda_p$. Lemma 3.3 could have been obtained as a corollary of this theorem. Furthermore, note that from the optimality of the Ritz values it follows that there is no real difference in writing $\widetilde{\theta} = -\infty$ from $\widetilde{\theta} = \infty$ if $\widetilde{\theta}^{-1} = 0$.

Kahan derived an explicit matrix with only eigenvalues at the end points of the intervals. This matrix can be used to compute the harmonic Ritz values, which can offer computational advantages, for example, when $\mathcal{V}$ is a Krylov subspace. See [16],[17, Section 10.5] for details.

Although the harmonic Ritz values provide optimal information about the spectrum of A, their convergence speed can be too slow for practical purposes, see also the a priori error bounds in Section 5. Several authors note (i.e. [14, 21, 15]) that "better" eigenvalue estimates are given by the so-called ρ-values

$$\rho_i \equiv \rho(\widetilde{u}_i) = \widetilde{u}_i^T A \widetilde{u}_i.$$

We note that for $\sigma = 0$ and $\lambda_{p-1} < 0 < \lambda_p$,

$$\rho_1 \widetilde{\theta}_1 = \|A\widetilde{u}_i\|_2^2 \geq \lambda_p^2 > 0,$$

and

$$0 = \sigma \leq \rho_1 = \frac{(\widetilde{u}_1^T A \widetilde{u}_1)^2}{\widetilde{u}_1 A \widetilde{u}_1} \leq \frac{\widetilde{u}_1^T A^2 \widetilde{u}_1}{\widetilde{u}_1 A \widetilde{u}_1} = \widetilde{\theta}_1.$$

The second inequality follows from an application of Cauchy-Schwarz. By generalizing this argument it easily follows that the ρ-value is always between the shift σ and the corresponding harmonic Ritz value. This was also observed by Morgan and Zeng, who derived this as a corollary of the following lemma. This lemma from [15] allows for a cheap calculation of the norm of the residu of a harmonic Ritz vector.

Lemma 3.4 (Morgan, Zeng [15, Theorem 2.1]). *Let* $r_i = A\widetilde{u}_i - \rho_i\widetilde{u}_i$, *then*

$$\|r_i\|_2^2 = (\rho_i - \sigma)(\widetilde{\theta}_i - \rho_i). \tag{5}$$

Proof. Using the fact that $(A - \widetilde{\theta}_i I)\widetilde{u}_i \perp (A - \sigma I)\widetilde{u}_i$ and $(A - \rho_i I)\widetilde{u}_i \perp \widetilde{u}_i$ leads to

$$\|r_i\|_2^2 = (A\widetilde{u}_i - \rho_i\widetilde{u}_i)^T(A\widetilde{u}_i - \rho_i\widetilde{u}_i) = (A\widetilde{u}_i - \widetilde{\theta}_i\widetilde{u}_i)^T(A\widetilde{u}_i - \rho_i\widetilde{u}_i)$$
$$= (A\widetilde{u}_i - \theta_i\widetilde{u}_i)^T(\sigma\widetilde{u}_i - \rho_i\widetilde{u}_i) = (\rho_i\widetilde{u}_i - \widetilde{\theta}_i\widetilde{u}_i)^T(\sigma\widetilde{u}_i - \rho_i\widetilde{u}_i) = (\rho_i - \sigma)(\widetilde{\theta}_i - \rho_i).$$

□

We note that the expression in (5) is very natural given the results of Temple, e.g. [2, Lemma 1.27] and [3, pp. 116].

4 A comparison with refined Rayleigh-Ritz

It is needless to say that it is of practical interest to have some understanding of how the shift σ influences the quality of the computed harmonic Ritz vectors. In this section we try to give some heuristics on this subject by restricting us to the harmonic Ritz values closest to the shift.

We assume that the eigenpair (λ_p, x_p) is of interest. For Rayleigh-Ritz with subspace $\mathcal{V}$ on the operator $(A - \sigma I)^{-1}$, picking σ close to the eigenvalue λ_p results in a good eigenvector approximation. The reason is that the spread/gap ratio, for example, for $\sigma < \lambda_p$,

$$\frac{\lambda_{p-1} - \lambda_p}{\lambda_{p+1} - \lambda_p}\,\frac{\lambda_{p+1} - \sigma}{\lambda_{p-1} - \sigma} \to 1 \text{ if } \sigma \to \lambda_p.$$

Theorem 2.1 from [19] now gives that the Ritz vector approaches the projection of x_p on $\mathcal{V}$, which is optimal. In harmonic Rayleigh-Ritz, however, we work with the space $(A - \sigma I)\mathcal{V}$. If σ is close to λ_p the approximation of x_p in $(A - \sigma I)\mathcal{V}$ is very poor. On the other hand, if σ is chosen at some distance from λ_p, Rayleigh-Ritz on $(A - \sigma I)^{-1}$ becomes less effective. In this section, we try to give some heuristics on how the quality of the harmonic Ritz vector depends on the choice of the shift σ. We do this by using a relation with the refined Rayleigh-Ritz method, a different method for constructing eigenvector approximations for interior eigenvectors popularized by Jia [8].

We first give a formal definition of refined Rayleigh-Ritz. Let τ be a given approximate eigenvalue for which we want an approximation for the corresponding eigenvector. Now, we define

$$\nu_\tau \equiv \min_{u\in\mathcal{V},\|u\|_2=1} \|Au - \tau u\|_2 \quad \text{and} \quad \widehat{u} \equiv \text{minarg}_{u\in\mathcal{V},\|u\|_2=1}\|Au - \tau u\|_2.$$

Therefore, $\widehat{u}$ can be viewed as the Ritz vector with smallest Ritz value of $(A - \tau I)^2$ with respect to $\mathcal{V}$, see (2). The vector $\widehat{u}$ is called the *refined Ritz vector* of A with respect to the approximate eigenvalue τ and the search subspace $\mathcal{V}$.

We use the following observation. If the approximate eigenvalue τ is in the middle of the interval with endpoints σ and $\widetilde{\theta}$ $(= \widetilde{\theta}_{\pm 1})$, then the refined Ritz vector $\widehat{u}$ and the harmonic Ritz vector $\widetilde{u}$ (with harmonic Ritz value $\widetilde{\theta}$) coincide as we will show in the theorem below. Moreover, the radius of the interval is exactly equal to the residual norm ν_τ of the refined Ritz vector: Fig. 1 illustrates this situation. This latter observation was also used by Lehmann in

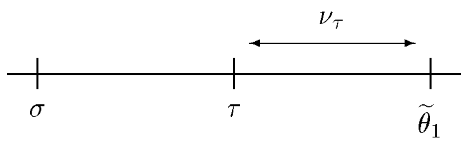


Figure 1: The location of the shift σ and the approximate eigenvalue τ for which the harmonic Ritz vector and the refined Ritz vector coincide (see Theorem 4.1).

a more general form in the construction of his optimal intervals [11, pp. 258] (see also [17, pp. 219]). The situation of Fig. 1 can be enforced for a given shift σ by selecting τ as the average of σ and $\widetilde{\theta}$, and, for given τ, by selecting σ at distance ν_τ from τ.

Theorem 4.1. *If σ is given, then select $\tau = \frac{1}{2}(\sigma + \widetilde{\theta}_{\pm 1})$. If τ is given, then select $\sigma = \tau \mp \nu_\tau$. Then, in both cases, we have that $\widetilde{\theta}_{\pm 1} = \tau \pm \nu_\tau$, $\nu_\tau = |\frac{1}{2}(\sigma - \widetilde{\theta}_{\pm 1})|$ and if $\widetilde{u}_{\pm 1}$ and $\widehat{u}$ are unique (up to a scalar), $\widehat{u}$ equals $\widetilde{u}_{\pm 1}$ up to a scalar.*

Proof. We work out the details for $\widetilde{\theta} = \widetilde{\theta}_1$. Consider a $v \in \mathcal{V}$ and put $\widetilde{\tau} \equiv \frac{1}{2}(\sigma + \widetilde{\theta})$ and $\gamma \equiv \frac{1}{2}(\widetilde{\theta} - \sigma)$. Then $v = \widetilde{u}$ iff $Av - \widetilde{\theta}v \perp (A - \sigma I)\mathcal{V}$, or equivalently,

$$(A - \sigma I)(A - \widetilde{\theta} I)v = (A - \widetilde{\tau} I)^2 v - \gamma^2 v \perp \mathcal{V}. \tag{6}$$

Note that $\gamma^2 = (\widetilde{\theta} - \sigma)^2/4 = \|(A - \widetilde{\tau} I)v\|_2^2$. Hence, $\widetilde{u}_1$ satisfies (2). It must also correspond to the smallest Ritz value, otherwise this would contradict the optimality of the Lehmann interval from Proposition 3.1.

Furthermore, $v = \widehat{u}$ iff

$$(A - \tau I)^2 v - \delta v \perp \mathcal{V} \tag{7}$$

for δ as small as possible. Note that (7) implies that $\delta = \|(A - \tau I)v\|_2^2 = \|(A - \tau I)\widehat{u}\|_2^2 = \nu_\tau^2$.

Now, using the fact that (6) and (7) are equivalent for appropriate scalars τ, $\widetilde{\tau}$, γ and δ, the theorem follows. $\square$

One nice consequence of this theorem is that for symmetric matrices it gives a method to compute the roots of the refined Ritz polynomial: pick $\sigma = \tau - \nu_\tau$, then the roots are given by the harmonic Ritz values, excluding the one at $\sigma + 2\nu_\tau$. This can be an alternative for the construction in Theorem 3.1 in [7].

Theorem 4.1 allows us to interpret the harmonic Ritz vector as a refined Ritz vector with shift $\widetilde{\tau} \equiv (\sigma + \widetilde{\theta})/2$ and using this interpretation we can try to explain some observed differences in the behavior of both methods with respect to the quality of the eigenvector approximation that is produced. We do this in Section 4.2.

4.1 The influence of τ on the quality of the refined Ritz vector

The term "quality" in the title of this section indicates the angle between the refined Ritz vector and the unknown eigenvector (x_p). For matrices that are non-normal it is necessary to choose τ close to the eigenvalue of interest, but in our situation the singular and eigenvectors coincide, and it is unclear what shift τ is best. In general it is difficult to make rigorous statements about this because the quality depends not only on eigenvalue distribution but also on the structure of the space $\mathcal{V}$. However, some general observations can be made. For example, if τ does not depend on $\mathcal{V}$ and is such that λ_p is the closest eigenvalue to τ then, for small enough ϵ ($\equiv \sin^2 \angle(x_p, \mathcal{V})$), we have the following sharp error bound for the refined Ritz vector.

Proposition 4.1. *Let*

$$\tau \in \left(\frac{1}{2}(\lambda_{p-1} + \lambda_p), \frac{1}{2}(\lambda_p + \lambda_{p+1})\right)$$

and $q \equiv \mathrm{argmin}_{i \neq p} |\lambda_i - \tau|$, $r \equiv \mathrm{argmax}_i |\lambda_i - \tau|$ *and* $\epsilon \equiv \sin^2 \angle(\mathcal{V}, x_p)$.
If

$$\epsilon < C_\tau^{-1}, \tag{8}$$

then we have for all $k \in \{2, \ldots, n-1\}$*:*

$$\sin^2 \angle(\widehat{u}, x_p) \leq \frac{1}{2}(1+\epsilon) - \frac{1}{2}\sqrt{(1-\epsilon)^2 - \kappa_\tau \epsilon}, \tag{9}$$

with

$$\kappa_\tau \equiv C_\tau + C_\tau^{-1} - 2 \quad \textit{and} \quad C_\tau \equiv \frac{(\lambda_r - \tau)^2 - (\lambda_p - \tau)^2}{(\lambda_q - \tau)^2 - (\lambda_p - \tau)^2}. \tag{10}$$

Furthermore, bound (9) is sharp.

Proof. Apply Theorem 3.1 from [19] to $(A - \tau I)^2$. □

The constant C_τ can be interpreted as a condition number (see [2, Section 2.3]) for the eigenvector x_p of the matrix $(A - \tau I)^2$. Hence, the choice of the shift τ affects this condition number. IFrom the fact that $C_\tau \geq 1$ and $\kappa_\tau \equiv C_\tau + C_\tau^{-1} - 2$ it follows that without additional information the shift $\tau = \tau^*$ that minimizes C_τ, results in the smallest attainable upper bound and gives this bound the largest area of application.

If we take into account the different choices for λ_q and λ_r in Proposition 4.1, then some simple analysis shows that the shift

$$\tau^* = \frac{\lambda_{p+1} + \lambda_{p-1}}{2} \tag{11}$$

minimizes C_τ and, therefore, without further information , is the best shift. Note that with $\tau = \tau^*$ the eigenvalues λ_{p-1} and λ_{p+1} after shifting and squaring become one double eigenvalue. Another consequence is that picking $\tau \approx \lambda_p$ is only expected to be optimal if the eigenvalue distribution is uniform around λ_p.

We expect that (11) is, in general also a very good choice for larger values of ϵ. But, additionally, if $\mathcal{V}$ does not contain fairly good approximations for the eigenvectors with eigenvalues close to λ_p, we often see that the choice of τ becomes relatively less important. This is illustrated by Figure 2 (Left picture) for the matrix $A = \mathrm{diag}(1, 2, \ldots, 100, 110, 114, \ldots, 200)$ and $\lambda_p = 110$. We have applied k iterations Lanczos with a starting vector with all components equal and computed the refined Ritz vector for various choices of τ. For this matrix we expect from (11) that $\tau = 107$ is a good choice while the real minimum value, τ^*, is close to this value. For the Lanczos method with more general matrices we see that the shift τ^* lies more in the direction of $\lambda_{p\pm1}$ if $x_{p\pm1}$ is relatively well represented in $\mathcal{V}$.

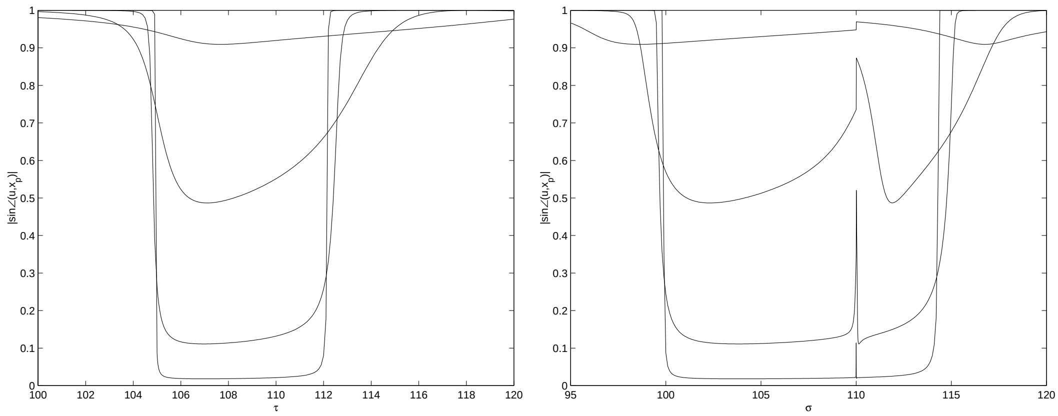


Figure 2: Left picture: The sine of the angle between the refined Ritz vector and x_p. Right picture: The sine of the angle between the harmonic Ritz vector ($\widetilde{u}_1$ if $\tau > 110$ and $\widetilde{u}_{-1}$ otherwise) and x_p. In both cases for $k = 25, 50, 75, 100$ iterations Lanczos and for all lines a smaller minimum value indicates more iterations Lanczos.

4.2 The influence of σ on the quality of a harmonic Ritz vector

We are now in a position to translate the observations in the previous section to the harmonic Ritz method using Theorem 4.1. First, if $\widetilde{\theta}$ is far from λ_p, then the shift $\widetilde{\tau} \equiv (\sigma + \widetilde{\theta})/2$ can be at some distance from τ^*. This is not necessarily a problem but can cause that the refined Ritz approach picks up information about x_p a little faster, see also the second experiment in Section 8.

If τ^* is the best shift for the refined Ritz approach then the harmonic Ritz vector corresponding to $\widetilde{\theta}_{\pm 1}$ is the best possible approximation for x_p if and only if $\sigma^* = \tau^* \mp \nu_{\tau^*}$. On the other hand if $\epsilon \to 0$ then $\nu_{\tau^*} \to |\lambda_p - \tau^*|$. Hence, we expect the optimal shifts σ^* to become arbitrary close to λ_p and $2\tau^* - \lambda_p$. More precisely, if τ^* is a bounded number, then $\nu_{\tau^*} = O(\sqrt{\epsilon})$ and the optimal shifts lie asymptotically at $\lambda_p + O(\sqrt{\epsilon})$ and $2\tau^* - \lambda_p + O(\sqrt{\epsilon})$. So, if no additional information is at hand the optimal shifts for the harmonic Rayleigh-Ritz method are at

$$\sigma^* = \lambda_{p-1} + \lambda_{p+1} - \lambda_p + O(\sqrt{\epsilon}) \text{ and } \lambda_p + O(\sqrt{\epsilon})$$

for ϵ small enough.

The right picture in Figure 2 shows this. There are two optimal values for σ that are becoming arbitrary close to $\lambda_p = 110$ and $2\tau^* - \lambda_p \approx 104$ when the number of Lanczos iterations increases. Although the optimal shift becomes closer and closer to $\lambda_p = 110$, the shift $\sigma = 110$ is not a very good candidate.

From our reasoning it is clear that comparing the quality of the refined Ritz and a certain harmonic Ritz vector for $\widetilde{\theta} \to \lambda_p$ amounts to comparing the shifts τ and $\widetilde{\tau} = (\sigma + \lambda_p)/2$. Which methods works best depends on $\mathcal{V}$ and the distribution of the eigenvalues and differs from situation to situation.

One of the advantages of the harmonic Rayleigh-Ritz method is that, with this shift for x_p, it can also provide good approximations for the eigenvector x_{p-1}. For the refined Ritz method a good shift, like in (11), introduces a double eigenvalue and therefore potentially a poor approximation for x_{p-1} or x_{p+1}. This seems less likely for the harmonic Rayleigh-Ritz method (and somehow easier to detect). See also the numerical experiments and conclusion in [14]. The harmonic Ritz values provide valuable information about the spectrum of the matrix, which is of course also an advantage.

5 A priori error estimation

For the Rayleigh-Ritz method the *a priori* error bounds

$$\theta_1 - \lambda_1 \leq (\lambda_n - \lambda_1) \sin^2 \angle(\mathcal{V}, x_1) \tag{12}$$

and

$$\sin^2 \angle(u_1, x_1) \leq \frac{\theta_1 - \lambda_1}{\lambda_2 - \lambda_1} \;\Rightarrow\; \tan^2 \angle(u_1, x_1) \leq \frac{\theta_1 - \lambda_1}{\lambda_2 - \theta_1} \tag{13}$$

are standard bounds for the smallest Ritz value and the corresponding Ritz vector [10] . The first estimate is a consequence of the optimality property of the Ritz values. We translate (12) and (13) to the harmonic Rayleigh-Ritz method. Similar statements can be found in [14, Theorem 3].

For simplicity we, again, use that $\sigma = 0$ and the eigenvalue of interest is $\lambda_p > 0$. Of course, statements about the more general situation can be obtained by replacing $A \to \pm(A - \sigma I)$. Let $\tau \equiv \tan^2 \angle(x_p, \mathcal{V})$. We first give a variant of (13) for harmonic Ritz vectors.

Theorem 5.1. *Let* $q = \text{argmin}_{i \neq p} |\lambda_i - \widetilde{\theta}_1/2|$, *if there exists a harmonic Ritz value* $\lambda_p \leq \widetilde{\theta}_1 < \lambda_{p+1}$, *then*

$$\tan^2 \angle(\widetilde{u}_1, x_p) \leq \frac{\lambda_p(\widetilde{\theta}_1 - \lambda_p)}{\lambda_q(\lambda_q - \widetilde{\theta}_1)}.$$

Proof. According to Theorem 4.1 the pair $(\widetilde{\theta}_1^2/4, \widetilde{u}_1)$ is the Ritz pair of $(A - \widetilde{\theta}_1/2I)^2$ w.r.t. $\mathcal{V}$ with the smallest Ritz value. Now, apply the second bound in (13) . □

Besides the factor λ_p/λ_q (which can be less than one), the expression in this theorem is similar to the second bound in (13). But it is well known that the convergence of the harmonic Ritz values can be arbitrary slow. In fact it can even take some time before the first positive harmonic Ritz values pops up. This is easily illustrated. Let $u \equiv \sqrt{1-\epsilon}\, x_p + \sqrt{\epsilon}\, x_1$ with $\epsilon = \tau/(1+\tau)$. With $\mathcal{V} \equiv \text{span}(u)$, the value $\widetilde{\rho}(u)$ is the only harmonic Ritz value. We know that $0 < \widetilde{\rho}(u)$ iff $0 < \rho(u) = (1-\epsilon)\lambda_p + \epsilon\lambda_1$. Apparently, we may not expect that there are positive harmonic Ritz values if $\tan^2 \angle(x_p, \mathcal{V}) > -\lambda_p/\lambda_1$. The following theorem shows that for smaller angles, there is a positive harmonic Ritz value and gives an a-priori error estimate.

Theorem 5.2. *Consider a search space* $\mathcal{V}$. *If* $\tau \equiv \tan^2 \angle(\mathcal{V}, x_p) < -\lambda_p/\lambda_1$, *then there is a harmonic Ritz value* $\widetilde{\theta}_1$ *of* A *with respect to* $\mathcal{V}$ *for which*

$$0 \leq \widetilde{\theta}_1 - \lambda_p \leq \tau \max_i \frac{\lambda_i(\lambda_i - \lambda_p)}{\lambda_p + \tau\lambda_i}.$$

Proof. Let $x_{\mathcal{V}}$ be the normalized projection of x_p on $\mathcal{V}$. Decompose $x_{\mathcal{V}} = \sqrt{1-\epsilon}\, x_p + \sqrt{\epsilon}\, e$ with $e \perp x_p$ and $\|e\|_2 = 1$. Then $\rho(x_{\mathcal{V}}) > 0$ and $\lambda_p + \tau\lambda_1 > 0$. Hence, because $\tau = \epsilon/(1-\epsilon)$, we have

$$\widetilde{\rho} \equiv \widetilde{\rho}(x_{\mathcal{V}}) = \frac{(1-\epsilon)\lambda_p^2 + \epsilon e^T A^2 e}{(1-\epsilon)\lambda_p + \epsilon e^T A e} = \frac{\lambda_p^2 + \tau e^T A^2 e}{\lambda_p + \tau e^T A e}.$$

Therefore, $\lambda_p(\widetilde{\rho} - \lambda_p) = \tau e^T A(A - \widetilde{\rho} I)e \leq \tau\lambda_i(\lambda_i - \widetilde{\rho})$ with $i = 1$ (if $\widetilde{\rho} > \lambda_1 + \lambda_n$) or $i = n$ (otherwise), which implies $\widetilde{\rho} - \lambda_p \leq \lambda_i(\lambda_i - \lambda_p)/(\lambda + \tau\lambda_i)$. An application of Lemma 3.2 concludes the proof. $\square$

True a-priori bounds for small enough τ can be obtained by substituting the result of Theorem 5.2 in the bound of Theorem 5.1. This, shows that $\tan^2\angle(\widetilde{u}_1, x_p) = O(\tau)$ for $\tau \to 0$. Unfortunately, these bounds become more meaningless when λ_p lies closer to zero, because the convergence of $\widetilde{\theta}_1$ can be arbitrary slow for λ_p close to zero. Sharper asymptotic a-priori bounds can, for example, be obtained, by combining Theorem 4.1 with Proposition 4.1 or using a technique as used in [19] for the Rayleigh-Ritz method. However, this does not remove the problem of the small applicability for λ_p close to zero. The question is if this means that all harmonic eigenvectors can be poor approximations to x_p in some instances. If $\lambda_p = 0$, then all the eigenvectors of the pencil $[A, A^2]$ can have arbitrary components in the direction of x_p. This non-uniqueness seems to cause in (3) that many harmonic Ritz vectors can point in a direction close to x_p. Also, if τ is large compared to $|\lambda_p|$ this behavior is often observed, see [14]. It would be interesting to have an error bound for the harmonic Ritz vectors in case $\lambda_p = 0$ to better understand this behavior. Numerical experiments suggest that this upper bound only depends on the dimension of $\mathcal{V}$ and not on some measure of the gap as for $\lambda_p \neq 0$. In fact, we expect that there is a harmonic Ritz vector $\widetilde{u}$ such that $\tan^2\angle(\widetilde{u}, x_p) \leq k\tau$, in which case the angle between all harmonic Ritz vectors and x_p is equal, this seems similar as for Rayleigh-Ritz for larger angles, see [22]. However, we have no proof for this.

6 A posteriori error estimation

Useful information about the eigenvalues of a matrix can often be obtained by using projection techniques. When a subspace is given the best one can do is to obtain intervals in which at least one eigenvalue can be found. In iterative methods that use harmonic Rayleigh-Ritz, Lehmann's optimal intervals from Proposition 3.1 are obtained as a cheap by-product. However, the size of these intervals depends on the choice of the shift and they are in particular not very small. In this section we are interested in how to choose the shift σ such that we have the distance between $\widetilde{\theta}$ and σ as small as possible (in contrast to Section 4 where we gave a priori considerations for shifts that result in good eigenvector approximations). This means that we have located an eigenvalue with maximal precision, see Proposition 3.1. Another advantage of a small interval is illustrated in the next lemma.

Lemma 6.1. *Let $(\widetilde{\theta}, u)$ be a harmonic Ritz pair and ρ the corresponding ρ-value and define $r \equiv A\widetilde{u} - \rho\widetilde{u}$. Then*

$$2\|r\|_2 \leq |\widetilde{\theta} - \sigma|$$

with equality iff $\rho = (\widetilde{\theta} + \sigma)/2$.

Proof. From Lemma 3.4 it follows

$$4\|r\|_2^2 = 4(\rho - \sigma)(\widetilde{\theta} - \rho).$$

This expression is maximal for $\rho = (\widetilde{\theta} + \sigma)/2$. $\square$

From Lemma 6.1 we see that the harmonic Ritz vector corresponding to the harmonic Ritz value closest to the shift necessarily has a small residu and therefore has a small backward error. Hence, $\widetilde{\theta}$ cannot be a so-called *ghost eigenvalue*.

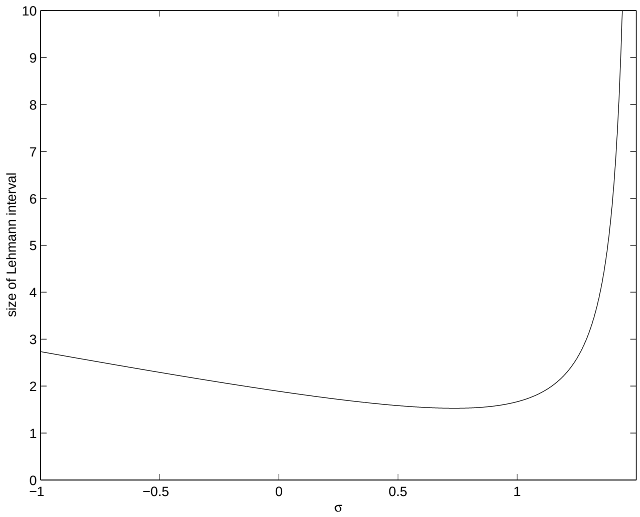


Figure 3: Size of Lehmann interval as a function of σ.

We call a shift σ^* best if the distance between the shift and the closest harmonic Ritz value $\widetilde{\theta}$ is as small as possible. For the sake of clarity we start with a simple example. A similar illustration can be found in [17, Section 10.5].

Example 6.1. Let the matrix A be 3 dimensional and diagonal with $A_{ii} = i$ and $\mathcal{V} = \text{span}(u)$ with $u = (1, 1/2, 1/2)^T$. The one harmonic Ritz value in this case is given by the harmonic Rayleigh quotient

$$\widetilde{\theta} = \widetilde{\rho}_\sigma(u) = \sigma + \frac{u^T(A - \sigma I)^2 u}{u^T(A - \sigma I)u}$$

and the only Ritz value is $\theta = \rho = 1.5$. Figure 3 shows the size of the Lehmann interval $|\widetilde{\theta} - \sigma|$ for some values of $\sigma < \theta$. A simple computation shows that the smallest interval is attained for $\sigma^* = \theta - \|Au - \theta u\|_2 \approx 0.74$ for which $|\widetilde{\theta} - \sigma| = 2\|Au - \theta u\|_2 \approx 1.53$. Note that there is of course a second minimal value at $\theta + \|Au - \theta u\|_2$.

Lemma 6.2. *The shift σ^* is best iff*

$$\sigma^* = {u^*}^T A u^* \pm \|Au^* - ({u^*}^T A u^*)u^*\|_2 \tag{14}$$

and u^* minimizes

$$\|Au^* - ({u^*}^T A u^*)u^*\|_2 \ . \tag{15}$$

Proof. According to Theorem 4.1 minimizing $|\widetilde{\theta} - \sigma|$ with respect to σ is equivalent to minimizing ν_τ with respect to τ. Since, $\|Au - (u^T A u)u\|_2 \le \|Au - \tau u\|_2$ for all normalized u and τ, we see that the claim follows. $\square$

In [17] it is remarked that no explicit expression is available for the best shift: considering the nonlinearity of (15) it is not likely that such an expression exists. The two conditions do, however, give a computable expression for the best shift. Note that this computation only requires the knowledge of the low dimensional matrices $V^T A^2 V$ and $V^T A V$ and can be done with a suitable iterative method. We propose a similar method for harmonic Rayleigh-Ritz by adapting the shift σ.

We now give a condition for, given a shift σ, computing a new shift, σ', that results in, at least, a smaller interval. The idea is as follows. Although the harmonic Ritz values provide the best upper bound on the eigenvalues closest to σ, they provide not better error estimates for the computed ρ-value than a simple application of the Bauer-Fike theorem [17, Theorem 4.5.1], see Lemma 6.1. Because in the Bauer-Fike interval ($[\rho - \|r\|_2, \rho + \|r\|_2]$) only information is used about the vector $\widetilde{u}$ it is suggested that we can find a smaller interval with the same inclusion property. In combination with Lemma 3.4 this suggests a way, given an interval with boundaries σ and $\widetilde{\theta}$, for creating an even smaller interval by adapting our shift to

$$\sigma' \equiv \rho - \sqrt{(\widetilde{\theta} - \rho)(\rho - \sigma)}. \tag{16}$$

Lemma 6.3. *Let σ' as in (16) and $\widetilde{\theta}'_1$ the smallest harmonic Ritz value w.r.t. to this shift for which $\widetilde{\theta}'_1 > \sigma'$. Then*

$$|\widetilde{\theta}'_1 - \sigma'| \leq |\widetilde{\theta} - \sigma|$$

with equality iff $\rho = (\widetilde{\theta} + \sigma)/2$.

Proof. If ρ is not precisely in the middle of the Lehmann interval then

$$(\widetilde{\theta}'_1 - \sigma')^2 \leq 4(\widetilde{\theta} - \rho)(\rho - \sigma) < (\widetilde{\theta} - \sigma)^2.$$

The first inequality follows from Theorem 4.1 applied to the one dimensional subspace $\widetilde{u}$ followed by the minmax property of harmonic Ritz values (Lemma 3.2). If ρ is precisely in the middle of the interval $\sigma = \sigma'$ which concludes the proof. □

Note that the intersection of the Bauer-Fike interval and the Lehmann interval is nonempty because ρ is in both intervals, on the other hand the Bauer-Fike interval cannot be strictly contained in the Lehmann interval, this would contradict the optimality from Proposition 3.1.

We now give a simple illustration of (16) for post-processing which aims at making optimal use of the information at hand ($\mathcal{V}$ and $A\mathcal{V}$).

6.1 A simple experiment

The matrix A is 10 dimensional and diagonal with on the diagonal $A_{ii} = i - 6$ for $i = 1, 2, \ldots, 10$. We are interested in a small interval containing at least one eigenvalue and preferably in the neighborhood of zero. As a subspace we generated a random, 4 dimensional space $\mathcal{V}$ with $\epsilon = \sin^2 \angle(\mathcal{V}, e_6)$ and computed the harmonic Ritz vectors with initial shifts $\sigma_{\texttt{start}} = -0.1$ and $\sigma_{\texttt{start}} = 0$. As initial interval we took the one with the harmonic Ritz value corresponding to the smallest residu and repeatedly computed the harmonic Ritz values according to the new shift (16). Tables 1 and 2 show the results for the two situations.

For $\sigma_{\texttt{start}} = -0.1$ a few steps give some improvement of the best known interval. However, for smaller ϵ the gain is small. For $\sigma_{\texttt{start}} = 0$ there is no small Lehmann interval and hence no guaranteed good approximation for the eigenvalue close to zero. But it turns out there is one. In this case the Bauer-Fike intervals show some more possibilities for improvement and a few steps remove the dependence of the initial approximation on the shift. In these experiments one or two steps seem to be sufficient.

ϵ	Step	σ	Bauer-Fike interval	size	Lehmann interval	size
0.1	0	-0.1000	[-0.5807,0.9072]	1.4879	[-0.1000,2.2656]	2.3656
	1	-0.5807	[-0.5894,0.8694]	1.4589	[-0.5807,0.8783]	1.4590
	2	-0.5894	[-0.5897,0.8692]	1.4589	[-0.5894,0.8694]	1.4589
	3	-0.5897	[-0.5897,0.8692]	1.4589	[-0.5897,0.8692]	1.4589
0.01	0	-0.1000	[-0.2271,0.2559]	0.4830	[-0.1000,0.5241]	0.6241
	1	-0.2271	[-0.2275,0.2549]	0.4824	[-0.2271,0.2553]	0.4824
	2	-0.2275	[-0.2275,0.2549]	0.4824	[-0.2275,0.2549]	0.4824
	3	-0.2275	[-0.2275,0.2549]	0.4824	[-0.2275,0.2549]	0.4824
0.001	0	-0.1000	[-0.0752,0.0779]	0.1532	[-0.1000,0.0592]	0.1592
	1	-0.0752	[-0.0752,0.0780]	0.1532	[-0.0752,0.0779]	0.1532
	2	-0.0752	[-0.0752,0.0780]	0.1532	[-0.0752,0.0780]	0.1532
	3	-0.0752	[-0.0752,0.0780]	0.1532	[-0.0752,0.0780]	0.1532

Table 1: Some numbers for $\sigma_{\texttt{start}} = -0.1$

7 Harmonic Rayleigh-Ritz and Lanczos

Krylov subspaces play an essential role in computational processes for eigenproblems. We assume in this section that the space $\mathcal{V}$ is a Krylov subspace, this makes that $AV - V(V^TAV)$ has rank one. The harmonic Ritz values in this situation are related to the roots of kernel polynomials, and hence with the convergence of iterative methods for linear systems like MINRES [16] and GMRES for non-Hermitian problems [6]. In this case the harmonic Ritz pairs seem to have some additional properties.

Lanczos is characterized by the following relation

$$AV = VT + \beta v e_k^T, \text{ where } T \equiv V^TAV \ . \tag{17}$$

The harmonic Ritz values w.r.t. shift $\sigma = 0$ can be interpreted as Ritz values for the Krylov space generated by A^{-1} with the starting vector $A^k b$, hence they are unique. Furthermore, if $\det(T) \neq 0$ the harmonic Ritz values interlace the Ritz values and zero [16],

$$\widetilde{\theta}_{-l} \leq \theta_1 \leq \widetilde{\theta}_{-(l-1)} \leq \ldots \leq \theta_l < 0 < \theta_{l+1} \leq \widetilde{\theta}_1 \leq \ldots \leq \widetilde{\theta}_{k-l} \ . \tag{18}$$

In Figure 4 we have reported the results for an experiment from [16]. The matrix A is diagonal with elements $\{-7, -5, -3, -1, 1, 3, \ldots, 91\}$ and the starting vector consists of all ones. The frequent stagnation in the convergence of the harmonic Ritz values is apparent. Note that this behavior is necessary to keep the harmonic Ritz values interlacing the Ritz values as in (18). These stagnation points seem to coincide with a Ritz value being close to zero. We analyze this a little further.

Suppose that in some iteration $\theta_j = 0$ for some j. Consider $\widetilde{z} = z_i - \alpha z_j$ for some $i \neq j$. Using (17) we get

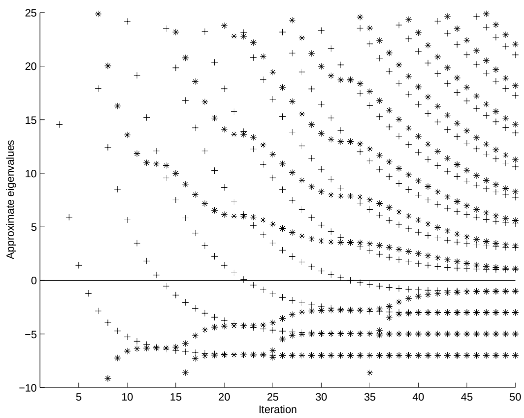
$$(AV)^T(AV)\widetilde{z} - \widetilde{\theta} V^TAV\widetilde{z} = \beta^2 e_k e_k^T z_i - \alpha\beta^2 e_k e_k^T z_j.$$

So, the pair $(V\widetilde{z}, \widetilde{\theta})$ defines a harmonic Ritz vector iff

$$\alpha \equiv \frac{e_k^T z_i}{e_k^T z_j}.$$

ϵ	Step	σ	Bauer-Fike interval	size	Lehmann interval	size
0.1	0	0.0000	[-0.5939,0.9599]	1.5538	[0.0000,3.4805]	3.4805
	1	-0.5939	[-0.5898,0.8691]	1.4589	[-0.5939,0.8650]	1.4589
	2	-0.5898	[-0.5897,0.8692]	1.4589	[-0.5898,0.8691]	1.4589
	3	-0.5897	[-0.5897,0.8692]	1.4589	[-0.5897,0.8692]	1.4589
0.01	0	0.0000	[-0.2459,0.2869]	0.5328	[0.0000,3.4805]	3.4805
	1	-0.2459	[-0.2276,0.2548]	0.4824	[-0.2459,0.2378]	0.4837
	2	-0.2276	[-0.2275,0.2549]	0.4824	[-0.2276,0.2548]	0.4824
	3	-0.2275	[-0.2275,0.2549]	0.4824	[-0.2275,0.2549]	0.4824
0.001	0	0.0000	[-0.0829,0.0870]	0.1699	[0.0000,3.4805]	3.4805
	1	-0.0829	[-0.0752,0.0779]	0.1532	[-0.0829,0.0710]	0.1539
	2	-0.0752	[-0.0752,0.0780]	0.1532	[-0.0752,0.0779]	0.1532
	3	-0.0752	[-0.0752,0.0780]	0.1532	[-0.0752,0.0780]	0.1532

Table 2: Some numbers for $\sigma_{\texttt{start}} = 0$



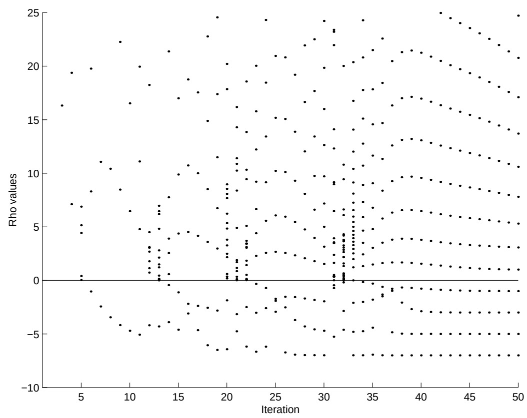


Figure 4: Left picture: harmonic Ritz values (*) and Ritz values (+), right picture shows the ρ-values

We can do this for all $i \neq j$, and if $e_k^T z_j \neq 0$ these vectors are linearly independent and are the harmonic Ritz vectors, together with u_j.

The ρ-values in this situation are

$$\rho = \frac{\theta_i}{\sqrt{1+\alpha^2}}. \tag{19}$$

So, if α is large the ρ-values are pushed towards 0. This appears to happen not very subtle. Since

$$\alpha^2 = \frac{\|Au_i - \theta_i u_i\|_2^2}{\|Au_j - \theta_j u_j\|_2^2}$$

this attraction towards zeros can be larger if the residual of the Ritz value on zero is relatively small. This probably explains that the behavior of the negative ρ-values in Figure 4 is less dramatic since, in this example, they are expected to correspond to more accurate approximations.

Because the harmonic Ritz values depend continuously on the shift we expect a similar behavior in case some Ritz value is close to zero. If $(V\widetilde{z}, \widetilde{\theta})$ is a harmonic Ritz pair we get by combining (3) and (17)

$$T(T - \widetilde{\theta} I)\widetilde{z} = -\beta^2 e_k (e_k^T \widetilde{z}) \ . \tag{20}$$

This shows that $\widetilde{z}$ is a multiple of $T^{-1}(T - \widetilde{\theta} I)^{-1} e_k$, hence

$$|\cos \angle(\widetilde{u}, u_j)| \sim \frac{\|Au_j - \theta_j u_j\|_2}{|\theta_j(\theta_j - \widetilde{\theta})|}$$

and $\widetilde{u}$ has relatively large components in the direction of the Ritz vectors with Ritz values close to $\widetilde{\theta}$ and zero. If a relative accurate Ritz vector is found ($\|Au_j - \theta u_j\|_2$ is small) the harmonic Ritz vectors have a small component in the direction of this Ritz vector or $|\theta_j(\widetilde{\theta} - \theta_j)|$ is small. Using this coefficients an expression for the corresponding ρ-value can be given, that suggests a similar behavior as for (19) for exact zero Ritz values.

In [1, Section 6] Beattie studied the stagnation points of *left-definite Lehmann bounds*, which give behavior similar to harmonic Ritz values. His explanation is based on an analog relation to (20) for left-definite Lehmann bounds. However, there is no mention of Ritz values being close to zero.

8 Numerical experiments

This section contains a few experiments with the harmonic Rayleigh-Ritz method related to the problem of selection. This means, that given a shift σ, we want to find a good approximation for the eigenpair closest to this shift (later we will consider the situation when the eigenvalue closest to the left or right of this shift is of interest).

Three conditions are considered. A straight-forward approach is to select the harmonic Ritz vector corresponding to the harmonic Ritz value closest to σ ($\min_i |\widetilde{\theta}_i - \sigma|$). We furthermore consider choosing the $\widetilde{u}_i$ for which $|\rho_i - \sigma|$ is smallest. A third selection condition is given by the smallest value of

$$(\rho_i - \sigma)(\widetilde{\theta}_i - \sigma). \tag{21}$$

Notice that since

$$(\rho_i - \sigma)(\widetilde{\theta}_i - \sigma) = \|A\widetilde{u}_i - \sigma \widetilde{u}_i\|_2^2,$$

this condition guarantees asymptotically correct selection. All three conditions can be applied cheaply. Because $|\rho_i - \sigma| \leq |\widetilde{\theta}_i - \sigma|$

$$(\rho_i - \sigma)^2 \leq (\rho_i - \sigma)(\widetilde{\theta}_i - \sigma) \leq (\widetilde{\theta}_i - \sigma)^2.$$

The first experiment illustrates some properties of these three selection methods. We searched for the eigenvalue $-1 < \mu < 1$ (closest to the origin) of the matrix

$$A = \begin{bmatrix} \mu & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ with } V = V_\phi \equiv \begin{bmatrix} \sqrt{1-\epsilon} & 0 \\ \sqrt{\epsilon}\sin(\phi) & -\cos(\phi) \\ \sqrt{\epsilon}\cos(\phi) & \sin(\phi) \end{bmatrix}.$$

Note that $\sin^2 \angle(\mathcal{V}, e_1) = \epsilon$. For a fixed ϵ we have applied harmonic Rayleigh-Ritz (zero shift) for a number of values of ϕ, applied the three selection conditions and calculated for the chosen

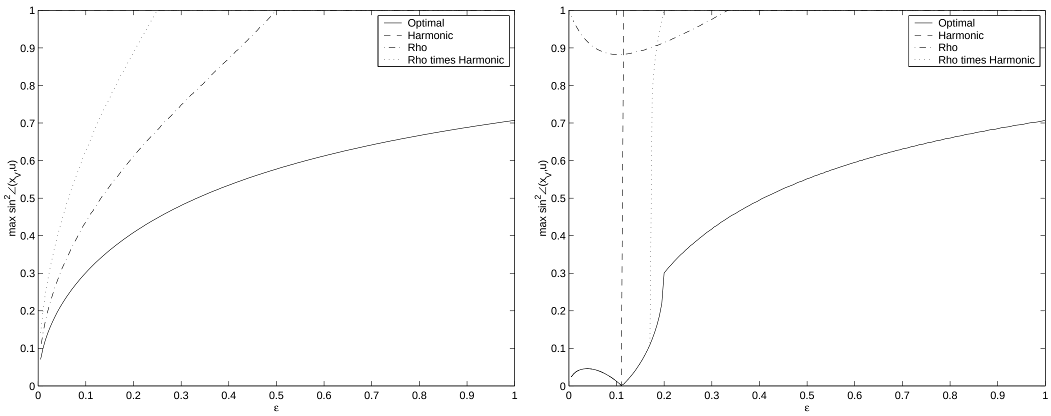


Figure 5: Numerical approximation of the maximal error over ϕ for the three different selection conditions and the theoretical situation the optimal approximation is selected for $\mu = 0$ (Left) and $\mu = -0.5$ (Right)

ϕ, the maximal angle between the selected harmonic Ritz vector and $x_{\mathcal{V}}$ (the projection of e_1 on $\mathcal{V}$). Doing this for a number of values for ϵ results in Figure 5.

From Section 5 it is clear that selection based on the harmonic Ritz value leads to correct selection asymptotically if σ is not equal to an eigenvalue. This can be seen from the figure for $\mu = -0.5$. In case $\mu = 0$ the graph for harmonic selection equals 1, this means that the selected harmonic Ritz vector can be perpendicular to $x_{\mathcal{V}}$ and this condition might perform very poorly in this situation.

For selection based on the ρ-values the situation is the reverse. When $\mu = 0$ the ρ-values provide useful information about the quality of the harmonic Ritz vector. However, if $\sigma \neq 0$ and some Ritz value is zero and this Ritz value is corresponding to a poor Ritz vector (i.e. ghost Ritz value), then this results in a zero ρ-value and therefore misselection. This can explain the phenomenon observed in the right picture. We expect ρ-selection not to be robust if σ is far from zero. Selection based on the product $\widetilde{\theta}\rho$ gives a reasonable compromise between the two conditions.

The second demonstration is adapted from an example in [14] and illustrates the use of harmonic Rayleigh-Ritz in the Davidson method [4]. We searched for the eigenvalue closest to 27.0 of the tridiagonal matrix A with $0.2, 0.4, \ldots, 58.8, 60.0$ on the diagonal and one on the sub- and super-diagonal. In every step of the solver the space $\mathcal{V}$ is expanded with a correction v given by the Davidson correction-equation

$$v = (\mathrm{diag}(A) - \sigma I)^{-1} r, \text{ with the residual } r \equiv (A\widetilde{u} - \rho\widetilde{u}).$$

Here $\widetilde{u}$ is the selected harmonic Ritz vector and ρ the corresponding ρ-value. Figure 6 shows the convergence history for the different selection conditions and the refined Ritz method.

The best strategy in this picture is the refined method with fixed shift although experiments show that the difference becomes small when σ becomes closer to 27.1. For $\sigma = 27.05$ the figure shows a very irregular behavior for the ρ-selection based method, the other two selection conditions perform equal. When σ is decreased to $\sigma = 27.0001$ the convergence for ρ-selection is still irregular but in the end not slower than for the $(\rho - \sigma)(\widetilde{\theta} - \sigma)$-selection. In the setting discussed here this is not really a problem, but misselection at restarts may be

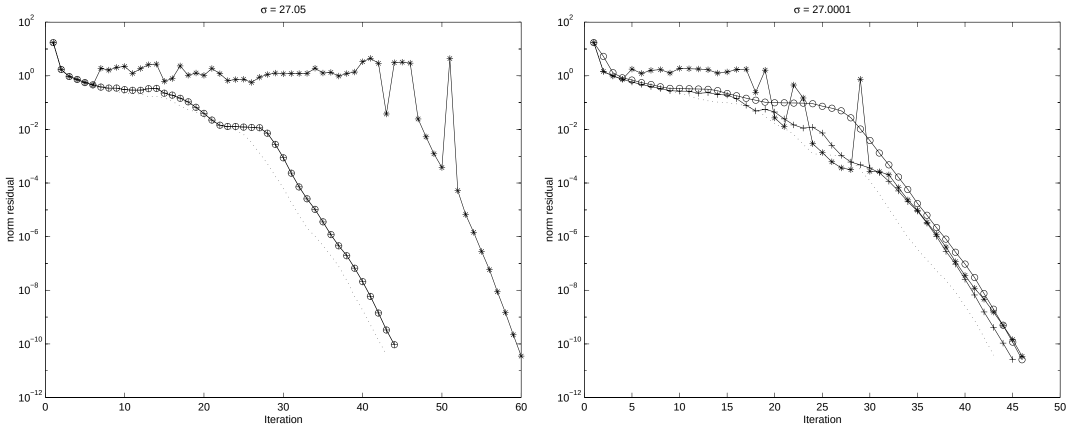


Figure 6: Finding the eigenpair with eigenvalue closest to σ with refined Ritz with shift σ (..) and harmonic Rayleigh-Ritz using harmonic selection (o), ρ-selection (*) and selection with (21) (+). Harmonic selection in the right picture finds the eigenvalue ≈ 27.2, which is not the eigenvalue closest to σ

fatal. The on harmonic selection based method converges to a different eigenpair, in contrast to the other methods.

Now we search for the largest eigenvalue smaller than σ, in other words the λ for which $1/(\sigma - \lambda_i)$ is maximal. It is not immediately clear how to adapt the refined Ritz method with fixed shift for this situation. The three conditions from our last experiment are adapted by selecting the harmonic Ritz vector, $\widetilde{u}_i$, for which $1/(\sigma - \widetilde{\theta}_i)$, $1/(\sigma - \rho_i)$ is maximal for the first two conditions. The third condition is changed to choosing the harmonic Ritz vector that maximizes

$$\frac{\operatorname{sign}(\sigma - \widetilde{\theta}_i)}{(\rho_i - \sigma)(\widetilde{\theta}_i - \sigma)}. \tag{22}$$

Figure 7 illustrates the results. Again, the convergence for ρ-selection is quite irregular. Selecting with harmonic Ritz values works in both situations, but again, if the shift is chosen any closer to 27 the methods finds the eigenvalue ≈ 26.8. The convergence for condition (22) is again smooth and robust in this situation. We conclude with the remark that (21) and (22) can also be used for non-normal problems.

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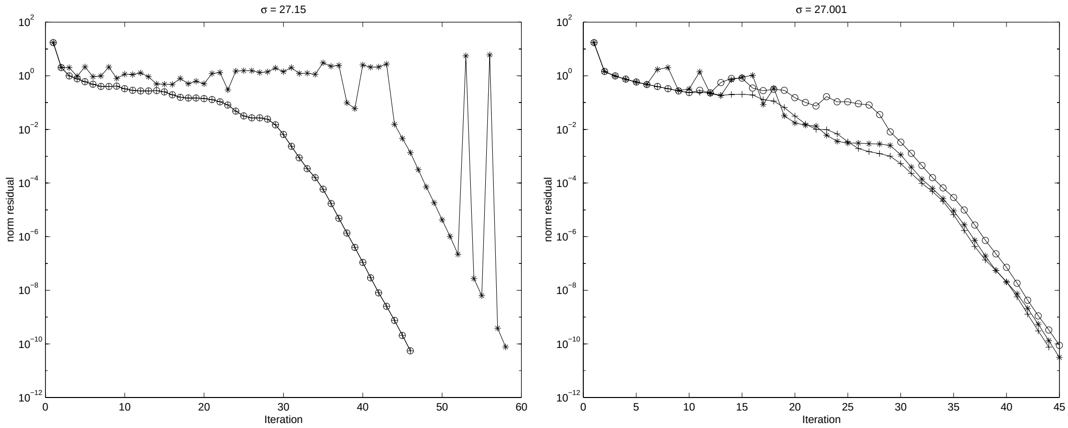

Figure 7: Finding the eigenpair with eigenvalue closest to and below σ with harmonic Rayleigh-Ritz using harmonic selection (o), ρ-selection (*) and selection with (22) (+). In all cases convergence is towards the desired eigenvalue

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