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Report

Author(s):
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Publication date:
2009

Permanent link:
https://doi.org/10.3929/ethz-a-006824950

Originally published in:
Technical Report / ETH Zurich, Department of Computer Science 610

HARMONIC RITZ VALUES AND THEIR RECIPROCALS

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Abstract. One application of harmonic Ritz values is to approximate, with a projection method, the interior eigenvalues of a matrix A while avoiding the explicit use of the inverse A^{-1}. In this context, harmonic Ritz values are commonly derived from a Petrov-Galerkin condition for the residual of a vector from the test space.

In this paper, we investigate harmonic Ritz values from a slightly different perspective. We consider a bounded functional ψ that yields the *reciprocals* of the harmonic Ritz values of a symmetric matrix A. The crucial observation is that with an appropriate residual s that differs from the commonly used one, many results from Rayleigh quotient and Rayleigh-Ritz theory naturally extend. The same is true for the generalization to matrix pencils (A, B) when B is symmetric positive definite.

These observations have an application in the computation of eigenvalues in the interior of the spectrum of a large sparse matrix. The minimum and maximum of ψ correspond to the eigenpairs just to the left and right of zero (or a chosen shift). As a spectral transformation, this distinguishes ψ from the original harmonic approach where an interior eigenvalue remains at the interior of the transformed spectrum. As a consequence, ψ is a very attractive vehicle for a matrix-free, optimization-based eigensolver such as the steepest descent, the nonlinear Preconditioned Conjugate Gradient (PCG), or the Locally Optimal Block PCG (LOBPCG) method. Instead of computing the smallest/largest eigenvalues by minimizing/maximizing the Rayleigh quotient, one can compute *interior* eigenvalues as the minimum/maximum of ψ.

AMS subject classifications. 65F15, 65Y15.

Key words. Rayleigh quotient, Ritz value, harmonic Ritz value, reciprocal, matrix-free computation, interior eigenpair, sparse iterative eigensolver, symmetric eigenproblem, generalized symmetric positive definite eigenproblem, preconditioned conjugate gradients, LOBPCG.

1. Introduction.

Prompted by the seminal works of Morgan [16], of Paige, Parlett, and van der Vorst [21], and of Sleijpen and van der Vorst [27], there has been a lot of recent research dedicated to the topic of harmonic Ritz values, see for example [2, 8, 10, 11, 13, 18, 26, 33] and also [1, Chapter 3] and [32, Chapter 4.4].

Harmonic Ritz values can rival the standard ones as approximation to the interior eigenvalues of a matrix. In this role, they have a natural place in iterative eigensolvers based on Rayleigh-Ritz principles, that is a matrix projection on a subspace which need not be of Krylov or block-Krylov type. Such methods include Lanczos [23, 29], (generalized) Davidson [4, 5, 17, 19], and Jacobi- Davidson [12, 15, 25, 27, 28, 30, 31].

While the harmonic Ritz values are commonly derived from a Petrov-Galerkin condition for the residual of a vector from the test space, this paper investigates them from a different angle. A first reward of this approach are some new, interesting results that one cannot easily obtain from the Petrov-Galerkin interpretation.

A second, from the practical point of view perhaps more important payoff is a functional whose extrema correspond to the eigenvectors belonging to the interior eigenvalues near zero, or a chosen shift. These can thus be computed by optimization methods such as (nonlinear) Preconditioned Conjugate Gradients (PCG) [3, 20, 24] and Locally Optimal Block Preconditioned Conjugate Gradients (LOBPCG) [14], by accessing A only in the form of a matrix-vector product, and without requiring the explicit or implicit evaluation of A^{-1}. Usually, these methods are used to compute

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the global minimum or maximum of the standard Rayleigh quotient, but they readily extend to spectral transformations.

This leads us back to our initial motivation for starting this current work, namely the desire to compute interior eigenvalues as harmonic Ritz values via PCG or LOBPCG. For a real symmetric matrix A, the standard Ritz values can be viewed as a matrix extension of the Rayleigh quotient

$$\rho(v) := \frac{v^t A v}{v^t v}, \ \ v \neq 0.$$

Likewise, one can see harmonic Ritz values as matrix extension of the functional

$$\phi(v) := \frac{v^t A^2 v}{v^t A v}, \ \ v \neq 0.$$

It was slightly disconcerting to note that ϕ is unbounded when A is indefinite, even in the case where it is nonsingular.

In addition, the harmonic ϕ is not practically useful for PCG and LOBPCG. These methods are designed to compute extremal values, that is either the minimum or maximum of the Rayleigh quotient or another suitable functional. However, the interior eigenvalues of A stay in the middle of the 'field of values' of ϕ.

Under these considerations, it seems more natural to instead consider the reversed version

$$\psi(v) := \frac{v^t A v}{v^t A^2 v}, \ \ v \neq 0.$$

This is the topic of Section 2. There, we also introduce the key definition of the associated residual

$$s(v) := v - Av\psi(v)$$

which features prominently in subsequent sections.

In addition to having a greater domain of definition, we found that ψ has some interesting features in common with ρ some of which are not shared by ϕ. In Section 3, we thus make the case that for both practical and theoretical reasons, ψ is a worthy subject of study itself.

In Section 4, we investigate extension of the functionals ρ, ϕ and ψ to subspaces. This leads to Ritz values and vectors. For the harmonic case, the Petrov-Galerkin condition on the residual that commonly is the fundamental definition follows here from the matrix functional. Attractive features of the matrix functional $\Psi(V)$ and the subspace residual $S(V)$ are illuminated.

Last but not least, Section 5 exhibits the generalization to matrix pencils (A, B) where B is symmetric positive definite. In this case, we study

$$\psi(v) := \frac{v^t A v}{v^t A B^{-1} A v}$$

with the associated generalized residual

$$s(v) := Bv - Av\psi(v).$$

Section 6 summarizes and gives a glimpse at the important practical application of ψ in optimization-based iterative eigensolvers.

2. Some rational quadratic forms. To set the scene, Section 2.1 summarizes basic properties of the Rayleigh quotient that can be found in [22, 23, 32]. The main point of Section 2.2 is to motivate the study of ψ which could be called the 'reversed harmonic Rayleigh quotient.'

2.1. Review of the Rayleigh quotient. Let A denote a real symmetric matrix. The Rayleigh quotient ρ of a vector $v \neq 0$ is defined as

$$\rho_A(v) := \frac{v^t A v}{v^t v}. \tag{2.1}$$

When there is no risk of ambiguity, the subscript mention of the matrix A is avoided.

THEOREM 2.1. *The Rayleigh quotient has three fundamental properties [23]:*

1. *Invariance under scaling: for real $\alpha \neq 0$: $\rho(\alpha v) = \rho(v)$.*
2. *Boundedness:*

$$\lambda_{\min}(A) = \min_{v \neq 0} \rho(v), \quad \lambda_{\max}(A) = \max_{v \neq 0} \rho(v), \tag{2.2}$$

   where $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ denote the smallest and largest eigenvalue of A, respectively.
3. *Stationarity: ρ is stationary in its argument v if and only if v is an eigenvector of A.*

Because of scaling-invariance, it is sufficient to consider ρ for vectors of unit length. For any such vector, ρ is a weighted average of the eigenvalues of A, this shows boundedness. Stationarity follows from inspection of the gradient

$$\nabla \rho(v) = 2\frac{Av - v\rho(v)}{v^t v} =: \frac{2}{v^t v} r(v). \tag{2.3}$$

Here,

$$r(v) := Av - v\rho(v) \tag{2.4}$$

denotes the residual which satisfies the Galerkin condition

$$r(v) \perp v. \tag{2.5}$$

By (2.2), one can compute the largest (or smallest) eigenvalues of A by an optimization method such as Preconditioned Conjugate Gradients [3, 20, 24]. In order to compute eigenvalues in the interior of the spectrum of A, one can replace A by a shifted-and-inverted version, that is apply the method to

$$\frac{v^t (A - \sigma I)^{-1} v}{v^t v}. \tag{2.6}$$

Here, the shift σ is assumed to be chosen close but not exactly equal to the eigenvalues of interest.

Why does one usually not consider the reversed Rayleigh quotient

$$\frac{v^t v}{v^t A v}? \tag{2.7}$$

The answer is: when A is indefinite, then $v \neq 0$ does not imply that $v^t A v \neq 0$. Thus the functional is unbounded, even if A is nonsingular. For example:

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = 0. \tag{2.8}$$

In this example, the problem does not seem to be very severe: the bisectors of the true eigenvectors are far away, in terms of the angle, from the vectors of interest. However, by considering a matrix $\mathrm{diag}(\alpha, -1)$, with $\alpha = 10^{-10}$ instead say, one sees that depending on the spectrum, the 'critical' vectors can be very close to an eigenvector which may, depending on the algorithm, make the computation challenging.

2.2. A harmonic functional and its reciprocal. In his pioneering paper [16], Morgan considers the inverse-free functional

$$\phi(v) := \frac{v^t(A-\sigma I)^2 v}{v^t(A-\sigma I)v} \tag{2.9}$$

for computing an interior eigenvalue close to σ. He proves that the eigenvector associated to the closest eigenvalue minimizes the magnitude of (2.9). Implicitly, this functional has been revisited by Paige, Parlett, and van der Vorst as it arises in their investigation of MINRES [21]. The authors point out among others the further occurrence in [7]. In [27], Sleijpen and van der Vorst generalize ϕ to a Petrov-Galerkin extraction approach for general subspaces. Further extensions are for example given in [2, 10, 11].

We now return to the functional (2.9), where for simplicity of notation we henceforth assume $\sigma = 0$. As the denominator generally is indefinite, the discussion at the end of Section 2.1 is relevant in the context of ϕ as well. From the computational point of view, it thus seems worthwhile to also consider the following functional

$$\psi_A(v) := \frac{v^t A v}{v^t A^2 v}. \tag{2.10}$$

When there is no risk of ambiguity, the subscript mention of the matrix A is again avoided and we use $\psi(v) := \psi_A(v)$. Of course, this is just the reversed version of (2.9), and for ease of notation, we do not mention σ. Nevertheless, as long as A is nonsingular, the denominator of (2.10) is definite and thus the functional is defined for any $v \neq 0$. Furthermore, we have the fundamental relation

$$\psi_A(v) = \rho_{A^{-1}}(w),\ w := Av. \tag{2.11}$$

We now investigate basic similarities between ρ, ϕ, and ψ.

THEOREM 2.2. *Let A be nonsingular, and consider ϕ from (2.9) with $\sigma = 0$, and $\psi = \psi_A$ as in (2.10).*

1. *For all v where ϕ is defined, one has $\phi(v) \cdot \psi(v) = 1$.*
2. *Both ϕ and ψ are invariant under scaling of the argument v.*
3. *ψ is bounded for $v \neq 0$.*

$$\lambda_{\min}(A^{-1}) = \min_{v\neq 0} \psi(v), \quad \lambda_{\max}(A^{-1}) = \max_{v\neq 0} \psi(v). \tag{2.12}$$

ϕ is only bounded if A is definite.

4. *ϕ and ψ are stationary if and only if v is an eigenvector of A.*

Proof. Scaling invariance is immediate. Without loss of generality, let $\|w\|_2 = 1$. Then $\alpha_i := w^t v_i$, $\sum \alpha_i^2 = 1$, and $v = \sum \alpha_i v_i$ imply that

$$\psi_A(v) = \sum \frac{\alpha_i^2}{\lambda_i(A)}. \tag{2.13}$$

Thus, ψ is a weighted average of the eigenvalues of A^{-1}. As A is nonsingular, the mapping $v \to w$ is one-to-one and (2.12) follows from (2.11) and (2.2). ϕ is unbounded when A is indefinite, compare the example at the end of Section 2.1. To prove stationarity, we note that

$$\nabla\phi(v) = 2\frac{A}{v^t A v}\left[Av - v\phi(v)\right]. \tag{2.14}$$

The last factor vanishes if and only if v is an eigenvector. Similarly,

$$\nabla\psi(v) = 2\frac{A}{v^t A^2 v}\left[v - Av\psi(v)\right]. \tag{2.15}$$

When v is an eigenvector, then the last factor vanishes. Conversely, assume that the factor vanishes. In this case ψ cannot be zero: cancellation is needed as $v \neq 0$ and $Av \neq 0$. Thus ϕ is defined, and using the first part of the theorem shows that also (2.14) must be zero, that is v is an eigenvector. □

The preceeding results show that where defined, one has for $v, \|Av\|_2 = 1$,

$$\frac{1}{\phi_A(v)} = \sum \frac{\alpha_i^2}{\lambda_i(A)}. \tag{2.16}$$

Hence, ϕ is a harmonic weighted average of the eigenvalues of A, motivating the name [21]. The last factor from (2.14) could be called the harmonic residual

$$r^{(h)}(v) := Av - v\phi(v). \tag{2.17}$$

It is defined wherever ϕ is defined and differs from the standard residual (2.4) only in the choice of the scaling factor for v. The Petrov-Galerkin condition

$$r^{(h)}(v) \perp Av \tag{2.18}$$

holds which, when A is definite, can be written as $r^{(h)}(v) \perp_A v$. (2.15)'s last factor,

$$s(v) := v - Av\psi(v) \tag{2.19}$$

is the residual with respect to ψ and defined for any $v \neq 0$. It also satisfies a Petrov-Galerkin condition

$$s(v) \perp Av. \tag{2.20}$$

The denominator $v^t A^2 v$ of (2.10) and the pre-factor of (2.15) suggests for ψ the normalization

$$\|Av\|_2 = \|v\|_{A^2} = 1, \tag{2.21}$$

using that A^2 induces a norm as long as A is nonsingular. This normalization is usually also used in the derivation of ϕ by a Petrov-Galerkin condition as it simplifies the resulting generalized eigenproblem to a standard one, see [1, page 41]. Which of the two norms from (2.21), Euclidean or A^2, to use best can depend on the situation and will slightly change the interpretation. From the Petrov-Galerkin point of view, one is interested in results on v as Av only matters as vector from a test space. On the other hand, for a nonlinear Preconditioned Conjugate Gradient method, the normalization with respect to A^2 is very natural as Section 3 illustrates. We return to the subject of metrics in Section 3.4. For the moment, we observe that neither ϕ nor ψ share the Rayleigh quotient's translation property $\rho_{A-\sigma I}() = \rho_A() - \sigma$, and that the normalization (2.21) is shift-dependent. Last, we note that (2.10) can also be interpreted as a fraction figuring the standard Rayleigh quotient ${}^{v^tAv}/_{v^tv}$ in the numerator and the 'folded' Rayleigh quotient ([16, 'Method 2'][36]) ${}^{v^tA^2v}/_{v^tv}$ in the denominator. This observation will play a significant role in Section 5.2 where ψ is generalized to pencils (A, B). There, $\psi_{(A,B)}(v) := {}^{v^tAv}/_{v^tAB^{-1}Av}$ which again is a quotient of standard ${}^{v^tAv}/_{v^tBv}$ and folded ${}^{v^tAB^{-1}Av}/_{v^tBv}$ Rayleigh quotients.

3. Similarities between ψ and ρ. We here formulate results for ψ similar to existing ones for ρ. While standard theory of harmonic Ritz values commonly considers the harmonic residual $r^{(h)}$, we here see the benefits of the use of s from (2.19). In judging the results, it is crucial to keep in mind that the residual and the error bounds do not require the evaluation of A^{-1} and are computable using A only.

3.1. Minimal residual properties. This short section points out a similarity between ρ, r and ψ, s that is not shared by $\phi, r^{(h)}$.

We first recall the following minimal residual property.

THEOREM 3.1. *[23, Fact 1.8] For a given vector v and any scalar σ holds*

$$\|r(v)\|_2 = \|Av - \rho(v)v\|_2 \le \|Av - \sigma v\|_2. \tag{3.1}$$

COROLLARY 3.2. *Let $v \neq 0$ and assume that its harmonic residual $r^{(h)}(v)$ from (2.17) is defined. Then*

$$\|r(v)\|_2 \le \|r^{(h)}(v)\|_2. \tag{3.2}$$

Remarkably, ψ and s enjoy a minimal residual property similar to the relation for ρ and r in Theorem 3.1.

THEOREM 3.3. *Let A be nonsingular. For a given vector v and any scalar σ, it holds for s from (2.19) that*

$$\|s(v)\|_2 = \|v - Av\psi(v)\|_2 \le \|v - Av\sigma\|_2. \tag{3.3}$$

Proof. At the end of Section 2.2 was noted that $s(v) \perp Av$. Hence

$$v - Av\sigma = [v - Av\psi(v)] - (\sigma - \psi(v))\, Av$$

is an orthogonal decomposition. This in turn yields

$$\|v - Av\sigma\|_2^2 = \|s(v)\|_2^2 + |\sigma - \psi(v)|^2 \|Av\|_2^2,$$

which proves the result. ☐

3.2. Backward error. It is remarkable that for a vector v of unit length, the norm of the standard residual $r(v)$ from (2.4) equals the norm of a rank-two perturbation of A that has $(\rho_A(v), v)$ as an eigenpair.

THEOREM 3.4. *[23, Theorem 4.5.2] Let $v \neq 0$, then $(\rho_A(v), v)$ is an eigenpair of $A - M$, where*

$$M = \frac{vr(v)^t + r(v)v^t}{\|v\|_2^2}, \ \|M\|_2 = \frac{\|r(v)\|_2}{\|v\|_2}. \tag{3.4}$$

Proof. Without loss of generality, assume that v is not an eigenvector, otherwise nothing needs to be shown. The eigenpair property follows from the Galerkin condition $r(v) \perp v$ and definition (3.4). To prove the second expression in (3.4), note that M has rank two and the eigenvectors belonging to its nonzero eigenvalues must be linear combinations of v and r. The Ansatz $x = \alpha v + \beta r$ yields

$$Mx = \frac{1}{\|v\|_2^2}\left(\beta(r^t r)v + \alpha(v^t v)r\right).$$

For the right-hand side to be collinear with x, one needs to have

$$\frac{\alpha^2}{\beta^2} = \frac{r^t r}{v^t v} \Leftrightarrow \frac{\alpha}{\beta} = \pm\sqrt{\frac{r^t r}{v^t v}}.$$

This yields the expression for $\|M\|_2$. ☐

Relation (2.11) between standard and reversed harmonic Rayleigh quotient

$$\psi_A(v) = \rho_{A^{-1}}(w),\ w := Av, \tag{3.5}$$

indicates that one can hope to find a similar result involving ψ.

THEOREM 3.5. *Let A be nonsingular, $v \neq 0$, and $s(v)$ as in (2.19). Then $(\psi_A(v), Av)$ is an eigenpair of $A^{-1} - N$, where*

$$N = \frac{Avs(v)^t + s(v)v^t A}{\|Av\|_2^2},\ \|N\|_2 = \frac{\|s(v)\|_2}{\|Av\|_2}. \tag{3.6}$$

Proof. If v is an eigenvector of A then $s(v) = 0$ and nothing is to show.

$$(A^{-1} - N)Av = v - NAv = v - s(v) = \psi_A(v)Av,$$

by the Petrov-Galerkin condition $s(v) \perp Av$. Comparison of (3.6) with (3.4) shows that $\|N\|_2$ can be computed in the same way as $\|M\|_2$ in the proof of Theorem 3.4. ☐

It seems difficult to find a similar relation for ϕ. While Theorem 3.5 is formulated in terms of a perturbation to A^{-1}, it can be readily stated in terms of a perturbation to the pencil (A, A^2) arising in the original definition (2.10) of ψ_A.

COROLLARY 3.6. *Let the conditions of Theorem 3.5 hold. Then v is a stationary point of the functional*

$$\frac{v^t(A - ANA)v}{v^t A^2 v}, \tag{3.7}$$

where N is defined in (3.6).

3.3. Distance bounds for eigenvalues. We now compare how the residual vectors introduced in Section 2.2 can be used in bounding errors in eigenvalues. A starting point is the following theorem of Weinstein's.

THEOREM 3.7. *[23, Theorem 4.5.1] For any scalar σ and any vector $v \neq 0$, there is an eigenvalue λ of A such that*

$$|\lambda - \sigma| \leq \frac{\|Av - v\sigma\|_2}{\|v\|_2}. \tag{3.8}$$

Two different proofs can be found in [23]. According to Theorem 3.1, the right hand side is minimized by $\|r(v)\|_2/\|v\|_2$.

COROLLARY 3.8. *Let $v \neq 0$, then*

1. *there is an eigenvalue* λ *of* A *such that*

$$|\lambda - \rho(v)| \leq \frac{\|r(v)\|_2}{\|v\|_2}, \tag{3.9}$$

2. *if* $v^t A v \neq 0$*, there is an eigenvalue* λ *of* A *such that*

$$|\lambda - \phi(v)| \leq \frac{\|r^{(h)}(v)\|_2}{\|v\|_2}. \tag{3.10}$$

Now, a Weinstein-type bound for s is established.

THEOREM 3.9. *Let* A *be nonsingular. For any scalar* σ *and any vector* $v \neq 0$*, there is an eigenvalue* $\lambda(A)$ *such that its reciprocal satisfies*

$$|\lambda^{-1} - \sigma| \leq \frac{\|v - Av\sigma\|_2}{\|Av\|_2}. \tag{3.11}$$

Proof.

$$\begin{aligned} \frac{\|v - Av\sigma\|_2^2}{\|Av\|_2^2} &= \frac{\|(A^{-1} - \sigma I)Av\|_2^2}{\|Av\|_2^2} \\ &= \rho_{(A^{-1}-\sigma I)^2}(Av) \\ &\geq \min_i \left(\lambda_i(A^{-1}) - \sigma\right)^2, \end{aligned}$$

where the last line exploits the bound from (2.2) on the standard Rayleigh-quotient. □

As discussed in Section 3.1, the right-hand side of the bound (3.11) is minimized by ψ. A second, sometimes better distance bound for eigenvalues is derived in Section 3.5.

3.4. Angle with the eigenvector. This Section gives an extension to the famous Davis-Kahan gap theorem [6, 23] for an inexact eigenpair.

For a given matrix A and $v \neq 0$, denote by $\bar{\lambda} = \bar{\lambda}(A)$ the eigenvalue closest to $\rho_A(v)$, and by $\bar{v}$ an associated eigenvector of unit length. With this notation, we have the following result.

THEOREM 3.10. *[23, Theorem 11.7.1] For a unit vector* v *with Rayleigh quotient* $\rho(v)$ *and residual* $r(v)$*, one has*

$$\frac{\|r(v)\|_2}{spread(A)} \leq |\sin\angle(v, \bar{v})| \leq \frac{\|r(v)\|_2}{gap(\rho(v), A)}, \tag{3.12}$$

where $gap(\rho, A) = \min\left\{|\rho - \lambda| : \lambda \neq \bar{\lambda}, \lambda \in spectrum(A)\right\}$ *and* $spread(A)$ *denotes the difference between the right- and left-most eigenvalues of* A*.*

Key to the proof is an orthogonal decomposition of v into the direction of the 'closest' eigenvector $\bar{v}$ and perpendicular to that. In the following proof, a similar decomposition

$$Av = \cos\vartheta\, A\bar{v} + \sin\vartheta\, Aw, \; A\bar{v} \perp Aw, \; \|A\bar{v}\|_2 = \|Aw\|_2 = 1. \tag{3.13}$$

is used. Here $\vartheta = \angle(Av, A\bar{v}) = \angle_{A^2}(v, \bar{v})$ and we come across the two different metrics already seen in (2.21).

THEOREM 3.11. *Let* A *be nonsingular. Let* $v \neq 0$ *such that* $\|Av\|_2 = 1$*, with* $\psi(v)$ *as in (2.10) and residual* $s(v)$ *as in (2.19). Denote by* $\bar{\lambda}^{-1}$ *the eigenvalue of* A^{-1}

closest to $\psi(v)$, and by $\bar{v}$ a corresponding eigenvector normalized such that $\|A\bar{v}\|_2 = 1$. Then one has

$$\frac{\|s(v)\|_2}{\mathit{spread}(A^{-1})} \leq |\sin\angle_{A^2}(v,\bar{v})| \leq \frac{\|s(v)\|_2}{\mathit{gap}(\psi(v),A^{-1})}. \tag{3.14}$$

Proof. First note that

$$s(v) = v - Av\psi(v) = (A^{-1} - \psi(v)I)Av.$$

Inserting here-in the orthogonal decomposition (3.13) one finds that

$$s(v) = \cos\vartheta\,(A^{-1} - \psi(v)I)A\bar{v} + \sin\vartheta\,(A^{-1} - \psi(v)I)Aw$$

is an orthogonal decomposition of s. This implies, with $\bar{\lambda}^2\|\bar{v}\|_2^2 = \|A\bar{v}\|_2^2 = 1$, that

$$\|s\|_2^2 = \cos^2\vartheta\,|\bar{\lambda}^{-1} - \psi(v)|^2 + \sin^2\vartheta\,\|(A^{-1} - \psi(v)I)Aw\|_2^2. \tag{3.15}$$

The upper bound in (3.14) follows from

$$\|(A^{-1} - \psi(v)I)Aw\|_2^2 \geq \min\rho_{(A^{-1}-\psi(v)I)^2} = \mathrm{gap}^2(\psi(v),A^{-1}).$$

For the lower bound, the condition $s(v) \perp Av$ and $\bar{\lambda}^2\|\bar{v}\|_2^2 = \|A\bar{v}\|_2^2 = 1$, yield

$$0 = \cos^2\vartheta\,\left(\bar{\lambda}^{-1} - \psi(v)\right) + \sin^2\vartheta\,w^tA(A^{-1} - \psi(v)I)Aw. \tag{3.16}$$

Multiply this by $\left(\bar{\lambda}^{-1} - \psi(v)\right)$ and subtract from (3.15) to find

$$\|s\|_2^2 = \sin^2\vartheta\,w^tA(A^{-1} - \psi(v)I)(A^{-1} - \bar{\lambda}^{-1}I)Aw. \tag{3.17}$$

Now apply the Cauchy-Schwarz inequality to find the lower bound in (3.14):

$$\|s\|_2^2 \leq \sin^2\vartheta\,\|A^{-1} - \psi(v)I\|_2\|A^{-1} - \bar{\lambda}^{-1}I\|_2 \leq \sin^2\vartheta\ \mathrm{spread}^2(A^{-1}).$$

□

Another useful consequence of (3.13) is that the error in ψ is proportional to the square of the error in v, analogous to the Rayleigh quotient.

THEOREM 3.12. *Let A be nonsingular. Let $v \neq 0$ such that $\|Av\|_2 = 1$, with $\psi(v)$ as in (2.10). Denote by $\bar{\lambda}^{-1}$ the eigenvalue of A^{-1} closest to $\psi(v)$ and let (3.13) be in force. Then, with $\vartheta = \angle_{A^2}(v,\bar{v})$:*

$$\begin{aligned} \psi(v) &= \cos^2\vartheta\ \psi(\bar{v}) + \sin^2\vartheta\ \psi(w) && (3.18)\\ &= \bar{\lambda}^{-1} - \sin^2\vartheta\ \left(\bar{\lambda}^{-1} - \psi(w)\right). && (3.19) \end{aligned}$$

3.5. Bound on the proximity of the closest eigenvalue. We assume the notation of Section 3.4 to be in force and present now a second distance bound for eigenvalues complementary to the one from Section 3.3.

THEOREM 3.13. *[23, Theorem 11.7.1] For a unit vector v with Rayleigh quotient $\rho(v)$ and residual $r(v)$, one has for the distance of $\rho(v)$ to the closest eigenvalue $\bar{\lambda}$:*

$$|\bar{\lambda} - \rho(v)| \leq \frac{\|r(v)\|_2^2}{\mathit{gap}(\rho(v),A)}. \tag{3.20}$$

The extended result is as follows.

THEOREM 3.14. *Let A be nonsingular. Let $v \neq 0$ such that $\|Av\|_2 = 1$, with $\psi(v)$ as in (2.10) and residual $s(v)$ as in (2.19). Denote by $\bar{\lambda}^{-1}$ the eigenvalue of A^{-1} closest to $\psi(v)$, and by $\bar{v}$ a corresponding eigenvector normalized such that $\|A\bar{v}\|_2 = 1$. Then one has*

$$|\bar{\lambda}^{-1} - \psi(v)| \leq \frac{\|s(v)\|_2^2}{gap(\psi(v), A^{-1})}. \tag{3.21}$$

Proof. Insert the basic identity $\cos^2\vartheta = 1 - \sin^2\vartheta$ into (3.16) to find

$$\sin^2\vartheta = \frac{\psi(v) - \bar{\lambda}^{-1}}{w^tA(A^{-1} - \bar{\lambda}^{-1}I)Aw}.$$

Now together with (3.17), this gives

$$\|s\|_2^2 = \left[w^tA(A^{-1} - \psi(v)I)(A^{-1} - \bar{\lambda}^{-1}I)Aw\right] \cdot \frac{|\psi(v) - \bar{\lambda}^{-1}|}{|w^tA(A^{-1} - \bar{\lambda}^{-1}I)Aw|}. \tag{3.22}$$

As $(A^{-1} - \psi(v)I)(A^{-1} - \bar{\lambda}^{-1}I)$ is symmetric positive-definite on $\bar{v}^\perp$, one finds

$$\begin{aligned} w^tA(A^{-1} - \psi(v)I)(A^{-1} - \bar{\lambda}^{-1}I)Aw &= \sum_i (\lambda_i^{-1} - \psi(v))(\lambda_i^{-1} - \bar{\lambda}^{-1})(w^tAv_i)^2 \\ &\geq \text{gap}(\psi(v), A^{-1}) \cdot |w^tA(A^{-1} - \bar{\lambda}^{-1}I)Aw|. \end{aligned}$$

□

3.6. Hessians. The Hessian of the Rayleigh quotient shows that the interior eigenvalues are in fact saddle points of ρ.

THEOREM 3.15. *[37] Let $v \neq 0$, then*

$$\nabla^2\rho(v) = \frac{2}{v^tv}\left\{\left(I - \frac{2}{v^tv}vv^t\right)(A - \rho(v)I)\left(I - \frac{2}{v^tv}vv^t\right)\right\}. \tag{3.23}$$

Proof. By (2.3)

$$\begin{aligned} \nabla^2\rho(v) &= \nabla\left(\frac{2}{v^tv}r(v)\right) \\ &= \nabla\left(\frac{2}{v^tv}\right)r(v)^t + \frac{2}{v^tv}\left\{(A - \rho(v)I) - \nabla(\rho(v))v^t\right\} \\ &= 2\frac{A - \rho(v)I}{v^tv} - 4\frac{r(v)v^t + vr(v)^t}{(v^tv)^2}. \end{aligned}$$

The last line equals (3.23) as $r(v) = (A - \rho(v)I)v \perp v$. □

It is interesting to note that the Hessian of ψ can be written using Householder reflectors.

THEOREM 3.16. *Let A be nonsingular and $v \neq 0$. If $w := Av$, then*

$$\nabla^2\psi(v) = \frac{2}{w^tw}A\left\{\left(I - \frac{2}{w^tw}ww^t\right)(A^{-1} - \psi(v)I)\left(I - \frac{2}{w^tw}ww^t\right)\right\}A. \tag{3.24}$$

Proof. By (2.15)

$$\nabla^2\psi(v) = \nabla\left(2\frac{A}{v^tA^2v}\left[v - Av\psi(v)\right]\right) = \nabla\left(2\frac{As}{v^tA^2v}\right)$$
$$= 2\frac{A-\psi(v)A^2}{v^tA^2v} - 4\frac{As(v)v^tA^2 + A^2vs(v)^tA}{(v^tA^2v)^2}.$$

Substitution of $s = (A^{-1} - \psi(v)I)Av$ yields

$$\nabla^2\psi(v) =$$
$$\frac{2}{v^tA^2v}A\left\{\left(A^{-1}-\psi(v)I\right) - 2\frac{\left(A^{-1}-\psi(v)I\right)Avv^tA + Avv^tA\left(A^{-1}-\psi(v)I\right)}{(v^tA^2v)}\right\}A. \tag{3.25}$$

This equals (3.24) as $v^tA\left(A^{-1}-\psi(v)I\right)Av = v^tAs(v) = 0$. □

4. Matrix functionals.

4.1. The matrix Rayleigh quotient. This section briefly reviews standard material that can be found for example in [23, Chapter 11], in [1, Chapter 3], or in [32, Chapter 4.4].

Let the columns of $V \in \mathcal{R}^{n\times k}$ be linearly independent. Define the matrix Rayleigh quotient

$$\varrho(V) := (V^tV)^{-1}V^tAV \tag{4.1}$$

As V^tV is nonsingular, it is even positive definite with a Cholesky factorization $V^tV = LL^t$. Thus $\varrho(V)$ is similar to the symmetric matrix $L^{-1}\varrho(V)L^{-t}$. Consequently, it has k real eigenvalues μ_i, the so-called Ritz values. These also are exactly the eigenvalues of the (definite) generalized symmetric eigenvalue problem

$$V^tAV\,y = \mu\,V^tV\,y,\ 0 \neq y \in \mathcal{R}^k. \tag{4.2}$$

Let y_i denote the eigenvector of (4.2) associated to μ_i. Then $Vy_i \in \mathcal{R}^n$ is called a Ritz vector.

In practice, one commonly chooses V to have orthonormal columns whenever possible. As this also allows for theoretical simplification, we henceforth assume that $V^tV = I$ and refer to [23, Section 11.10] for the more general setting. We note that $\mu_i = \rho(Vy_i)$ so that (4.2) can be rephrased as

$$0 = V^t\left[(A-\mu_iI)Vy_i\right] = V^tr(Vy_i) \tag{4.3}$$

to yield a Ritz-Galerkin condition stronger than (2.5).

As an extension of (2.4), one can also define the subspace residual

$$R(V) := AV - V\varrho(V). \tag{4.4}$$

It satisfies the subspace Galerkin condition

$$R(V) \perp V. \tag{4.5}$$

The subspace span(V) is invariant under A if and only if $R(V) = 0$.

4.2. Φ and Ψ: matrix versions of ϕ and ψ. Let A be nonsingular and the columns of $V \in \mathcal{R}^{n\times k}$ be linearly independent. The matrix versions of (2.9) and (2.10) are

$$\Phi(V) := (V^tAV)^{-1}V^tA^2V, \tag{4.6}$$

and

$$\Psi(V) := (V^tA^2V)^{-1}V^tAV, \tag{4.7}$$

respectively. When both Φ and Ψ are defined, they have real eigenvalues as they are similar to symmetric matrices. Since one has $\Phi(V)\Psi(V) = \Psi(V)\Phi(V) = I$, the eigenvalues of one are just the reciprocals of the other.

The eigenvalues μ_i of Φ are called the harmonic Ritz values. They are solutions of the (generally indefinite) generalized symmetric eigenvalue problem

$$V^tA^2V\,y = \mu\,V^tAV\,y,\ 0 \neq y \in \mathcal{R}^k. \tag{4.8}$$

Let the harmonic subspace residual

$$R^{(h)}(V) := AV - V\Phi(V), \tag{4.9}$$

then one has as the generalization of (2.18) that

$$R^{(h)}(V) \perp AV. \tag{4.10}$$

This Petrov-Galerkin condition is normally used to define the harmonic Ritz values and vectors, see for example [27] or [1, Chapter 3].

The blemish of Φ is that V^tAV need not be invertible for indefinite A, recall the example at the end of Section 2.1. This is not a negligible detail: for example, in [13], convergence of the harmonic Ritz values to an eigenvalue of A is shown under the condition that $\|(V^tAV)^{-1}\|$ is uniformly bounded. However, for interior eigenvalues of an indefinite (shifted) A, this condition might never be satisfied!

On the other hand, V^tA^2V is positive definite when A is nonsingular. This makes Ψ attractive. The associated definite generalized symmetric eigenvalue problem is

$$V^tAV\,y = \mu\,V^tA^2V\,y,\ 0 \neq y \in \mathcal{R}^k. \tag{4.11}$$

With

$$S(V) := V - AV\Psi(V) \tag{4.12}$$

one has the alternative Petrov-Galerkin condition

$$S(V) \perp AV. \tag{4.13}$$

One can ortho-normalize the columns of AV. In this case, (4.7) and (4.11) turn into a standard Rayleigh quotient and eigenproblem with the constraint $V^tA^2V = I$.

4.3. Similarities between Ψ and ϱ. Section 3 pointed out interesting parallels between ρ and ψ. We investigate here how some of them generalize to the matrix versions of the respective functionals. The focus is on results that involve Ψ and $S(V)$. In [26, Section 3], a nice summary of other similar features is given, including a translation of the Courant-Fischer Minmax/Maxmin principle.

First, we consider the generalization of the minimal residual properties from Section 3.1. For the matrix Rayleigh quotient, we have the following extension of Theorem 3.1.

THEOREM 4.1. *[23, Theorem 11.4.2] Let $V \in \mathcal{R}^{n\times k}$ with $V^tV = I$. Let $R(V)$ as in (4.4), then*

$$\|R(V)\|_2 = \|AV - V\varrho(V)\|_2 \leq \|AV - VB\|_2 \tag{4.14}$$

for any matrix $B \in \mathcal{R}^{k\times k}$.

We also find the following generalization of Theorem 3.3.

THEOREM 4.2. *Let A be nonsingular and $V \in \mathcal{R}^{n\times k}$ such that $V^tA^2V = I$. Then*

$$\|S(V)\|_2 = \|V - AV\Psi(V)\|_2 \leq \|V - AVB\|_2. \tag{4.15}$$

for any matrix $B \in \mathcal{R}^{k\times k}$.

Proof. We first note the auxiliary result

$$S(V)^tS(V) = V^tS(V) \tag{4.16}$$

which is a consequence of $S(V)^tS(V) = S(V)^tV + S(V)^tAV\Psi(V)$ and the Petrov-Galerkin condition (4.13). Now we have

$$\begin{aligned}(V - AVB)^t(V - AVB) &= V^tV - \Psi(V)^tB - B^t\Psi(V) + B^t(V^tA^2V)B \\ &= V^tS(V) + (\Psi(V) - B)^t\,(\Psi(V) - B)\end{aligned}$$

The matrix $(\Psi(V) - B)^t\,(\Psi(V) - B)$ is positive semidefinite. Weyl's Monotonicity Theorem [23, Theorem 10.3.1] yields that every eigenvalue, in particular the largest one, of $(V - AVB)^t(V - AVB)$ is greater or equal than the corresponding one of $V^tS(V)$. By (4.16), this completes the proof. □

As a generalization of Theorem 3.7, we have the next result.

THEOREM 4.3. *[23, Theorem 11.5.1] Let $V \in \mathcal{R}^{n\times k}$ with $V^tV = I$. Let $R(V)$ as in (4.4), then there are k eigenvalues $\lambda(A)$ such that for $i = 1, \dots, k$:*

$$|\lambda_{j_i}(A) - \mu_i(\varrho)| \leq \|R(V)\|_2. \tag{4.17}$$

For $\Psi(V)$ and $S(V)$, Theorem 3.9 generalizes to

THEOREM 4.4. *Let A be nonsingular and $V \in \mathcal{R}^{n\times k}$ such that $V^tA^2V = I$. Then there are k eigenvalues $\lambda(A^{-1})$ such that for $i = 1, \dots, k$:*

$$|\lambda_{j_i}(A^{-1}) - \mu_i(\Psi)| \leq \|S(V)\|_2. \tag{4.18}$$

Proof. Let $P := (AV, AW)$ such that $P^tP = PP^t = I$. The matrix $P^tA^{-1}P$ is orthogonally similar to A^{-1} and has the shape

$$P^tA^{-1}P = \begin{bmatrix} \Psi(V) & \\ & \Psi(W) \end{bmatrix} + \begin{bmatrix} & V^tAW \\ W^tAV & \end{bmatrix}.$$

To prove the result using again Weyl's Monotonicity Theorem [23, Theorem 10.3.1], one thus has to find $\|W^tAV\|_2$ which equals in magnitude the largest and smallest eigenvalue of the second term. For this, note that

$$P^tS(V) = \begin{bmatrix} V^tAV - V^tA^2V\Psi(V) \\ W^tAV - W^tA^2V\Psi(V) \end{bmatrix} = \begin{bmatrix} 0 \\ W^tAV \end{bmatrix}$$

using the definition of Ψ and $AV \perp AW$. Now, since $\|S(V)\|_2 = \|P^tS(V)\|_2 = \|W^tAV\|_2$, everything is shown. □

5. Matrix pencils. We consider here functionals for the matrix pencil (A, B) where A and B are real symmetric matrices, and B is also positive definite.

5.1. Generalized ρ. This review is intentionally brief, for background material see for example [23, Chapter 15] or [1, Chapter 5.7]. The (generalized) Rayleigh quotient ρ is defined as

$$\rho(v) := \rho_{(A,B)}(v) := \frac{v^t A v}{v^t B v}. \tag{5.1}$$

The gradient yields the residual

$$\nabla\rho(v) = 2\frac{Av - Bv\rho(v)}{v^t B v} =: \frac{2}{v^t B v} r(v). \tag{5.2}$$

Theorem 2.1 also holds in the generalized setting. The positive-definiteness of B implies existence of the Cholesky factorization $B = LL^T$. Thus, the pencils (A, B) and $(L^{-1}AL^{-t}, I)$ as well as (AB^{-1}, I) and $(B^{-1}A, I)$ have the same eigenvalues. Further, one can define for both $M := B$ and $M := B^{-1}$ an induced scalar product that yields the associated vector norm and angle:

$$(v, w)_M := w^t M v, \quad \|v\|_M := \sqrt{(v, v)_M}, \quad \angle_M(v, w) := \arccos\frac{|(v, w)_M|}{\|v\|_M \|w\|_M}.$$

One important application is that the eigenvectors of (A, B) can always be chosen B-orthonormal. Another one is the Galerkin condition $r(v) \perp v$. It can be written as

$$r(v) \perp_{B^{-1}} Bv. \tag{5.3}$$

The following Theorem 5.1 summarizes the beautiful extensions of the results in Section 3 to the generalized Rayleigh quotient.

THEOREM 5.1. *Let $v \neq 0$ be a vector and $\sigma \in \mathcal{R}$ a scalar.*

1. *Minimal residual property [23, Theorem 15.9.2]:*

$$\|r(v)\|_{B^{-1}} = \|Av - \rho(v)Bv\|_{B^{-1}} \le \|Av - \sigma Bv\|_{B^{-1}}. \tag{5.4}$$

2. *Backward error [1, Section 5.7.1]: $(\rho(v), v)$ is an eigenpair of $(A - M, B)$, where*

$$M = \frac{vr(v)^t + r(v)v^t}{\|v\|_2^2}, \ \|M\|_2 = \frac{\|r\|_2}{\|v\|_2}. \tag{5.5}$$

3. *Weinstein's bound [23, Theorem 15.9.1]: there is an eigenvalue λ of (A, B) such that*

$$|\lambda(A, B) - \sigma| \le \frac{\|Av - Bv\sigma\|_{B^{-1}}}{\|Bv\|_{B^{-1}}}. \tag{5.6}$$

4. *Angle with the closest eigenvector $\bar{v}$ [1, Section 5.7.1]:*

$$|\sin\angle_B(v, \bar{v})| = |\sin\angle_{B^{-1}}(Bv, B\bar{v})| \le \frac{\|r(v)\|_{B^{-1}}}{gap\,(\rho(v), (A, B))\ \|Bv\|_{B^{-1}}}, \tag{5.7}$$

with the straight-forward definition of the spectral gap as in Theorem 3.10.

5. *Hessian:*

$$\nabla^2\rho(v) = \frac{2}{v^t B v}\left\{\left(I - \frac{2}{v^t B v}Bvv^t\right)(A - \rho(v)B)\left(I - \frac{2}{v^t B v}vv^t B\right)\right\}. \tag{5.8}$$

Some results in Theorem 5.1 can be partly simplified using the normalization $\|v\|_B = \|Bv\|_{B^{-1}} = 1$.

5.2. Generalized ψ. In order to define ψ for pencils, we will again assume that A is nonsingular. Then, one way to extend ψ to the generalized case is via the fundamental relation (2.11) for the standard case, $\psi_A(v) = \rho_{A^{-1}}(Av)$. It can be applied to the pencil $(L^{-1}AL^{-t}, I)$ which is equivalent to (A, B) as noted in Section 5.1. This yields $(L^{-1}AL^{-t}, L^{-1}AB^{-1}AL^{-t})$ and the simpler, equivalent

$$\psi(v) := \psi_{(A,B)}(v) := \frac{v^t Av}{v^t AB^{-1}Av}. \tag{5.9}$$

Incidentally, it satisfies the fundamental relation

$$\psi_{(A,B)}(v) = \rho_{(A^{-1},B^{-1})}(w),\ w := Av. \tag{5.10}$$

Note that (λ, v) is an eigenpair of the pencil (A, B) if and only if $(1/\lambda, w)$ is an eigenpair of (A^{-1}, B^{-1}). The gradient of (5.9) guides the search for the definition of an appropriate residual:

$$\nabla\psi(v) = 2\frac{AB^{-1}}{v^t AB^{-1}Av}\left[Bv - Av\psi(v)\right]. \tag{5.11}$$

We let (5.11)'s last factor,

$$s(v) := Bv - Av\psi(v) \tag{5.12}$$

denote the (generalized) residual with respect to ψ. It is defined for any $v \neq 0$ and satisfies the Petrov-Galerkin condition

$$s(v) \perp_{B^{-1}} Av. \tag{5.13}$$

In generalization of (2.21), (5.9) and (5.11) suggest the normalization

$$\|Av\|_{B^{-1}} = \|v\|_{AB^{-1}A} = 1. \tag{5.14}$$

We are now ready to state the analogue to Theorem 5.1 for ψ.

THEOREM 5.2. *Let A be nonsingular, $v \neq 0$ be a vector and $\sigma \in \mathcal{R}$ be a scalar.*

1. *Minimal residual property:*

$$\|s(v)\|_{B^{-1}} = \|Bv - \psi(v)Av\|_{B^{-1}} \leq \|Bv - \sigma Av\|_{B^{-1}}. \tag{5.15}$$

2. *Backward error: $(\psi(v), Av)$ is an eigenpair of the pencil $(A^{-1} - N, B^{-1})$, where*

$$N = \frac{Avs(v)^t B^{-1} + B^{-1}s(v)v^t A}{\|Av\|_2^2},\ \|N\|_2 = \frac{\|B^{-1}s(v)\|_2}{\|Av\|_2}. \tag{5.16}$$

Equivalently, v is a stationary point of the perturbed functional

$$\frac{v^t(A - ANA)v}{v^t AB^{-1}Av}. \tag{5.17}$$

3. *Weinstein-type bound: there is an eigenvalue λ of (A, B) such that its reciprocal satisfies*

$$|\lambda^{-1} - \sigma| \leq \frac{\|Bv - Av\sigma\|_{B^{-1}}}{\|Av\|_{B^{-1}}}. \tag{5.18}$$

4. *Angle with the closest eigenvector $\bar{v}$: let $\vartheta = \angle_{B^{-1}}(Av, A\bar{v})$ and*

$$Av = \cos\vartheta\, A\bar{v} + \sin\vartheta\, Aw,\ A\bar{v} \perp_{B^{-1}} Aw,\ \|A\bar{v}\|_{B^{-1}} = \|Aw\|_{B^{-1}} = 1. \quad (5.19)$$

Then

$$\frac{\|s(v)\|_{B^{-1}}}{spread\,(A^{-1}, B^{-1})} \le |\sin\vartheta| \le \frac{\|s(v)\|_{B^{-1}}}{gap\,(\psi(v), (A^{-1}, B^{-1}))}. \quad (5.20)$$

5. *Error expansion for ψ: let (5.19) be in force, then*

$$\psi(v) = \bar{\lambda}^{-1} - \sin^2\vartheta\, \left(\bar{\lambda}^{-1} - \psi(w)\right). \quad (5.21)$$

6. *Proximity of ψ to the closest eigenvalue $\bar{\lambda}^{-1}$: with (5.19) in force, one has*

$$|\bar{\lambda}^{-1} - \psi(v)| \le \frac{\|s(v)\|^2_{B^{-1}}}{gap\,(\psi(v), (A^{-1}, B^{-1}))}. \quad (5.22)$$

7. *Hessian: let $w := Av$, then*

$$\nabla^2\psi(v) = \frac{2}{w^tB^{-1}w} A\left\{\left(I - \frac{2}{w^tB^{-1}w}B^{-1}ww^t\right)\left(A^{-1} - \psi(v)B^{-1}\right)\left(I - \frac{2}{w^tB^{-1}w}w(B^{-1}w)^t\right)\right\}A. \quad (5.23)$$

Proof. The Petrov-Galerkin condition (5.13) shows that

$$Bv - \sigma Av = s(v) + (\psi - \sigma)Av$$

is a B^{-1}-orthogonal decomposition. This is sufficient to show (5.15), see also the proof of Theorem 3.3.

The difficulty of the backward error result is to find the shape of N. With (5.16) at hand, one sees that

$$(A^{-1} - N)Av = v - B^{-1}s = \psi B^{-1}Av.$$

The rest of the proof proceeds as the ones in Section 3.2.

For proving (5.18), we first note that

$$Bv - \sigma Av = B(A^{-1} - \sigma B^{-1})Av.$$

Thus

$$\frac{\|Bv - Av\sigma\|^2_{B^{-1}}}{\|Av\|^2_{B^{-1}}} = \frac{(Av)^t(A^{-1} - \sigma B^{-1})B(A^{-1} - \sigma B^{-1})Av}{(Av)^tB^{-1}Av}. \quad (5.24)$$

One now needs the key insight that the right-hand side of (5.24) actually is the Rayleigh quotient of a 'folded' pencil, that is, its eigenvalues are exactly the squares of the eigenvalues of the pencil $(A^{-1} - \sigma B^{-1}, B^{-1})$. This in turn shows that the right-hand side is an upper bound on the squared distance to the closest eigenvalue, analogously to the proof of Theorem 3.9.

The proof of (5.20) becomes similar to the one of Theorem 3.11 when one substitutes orthogonality by B^{-1}-orthogonality. In analogy to (3.15), one finds

$$\|s\|^2_{B^{-1}} = \cos^2\vartheta\, |\bar{\lambda}^{-1} - \psi(v)|^2 + \sin^2\vartheta\, \|B(A^{-1} - \psi(v)B^{-1})Aw\|^2_{B^{-1}}. \quad (5.25)$$

With normalization (5.14), the equivalent of (3.16) becomes

$$0 = \cos^2 \vartheta \, \left(\bar\lambda^{-1} - \psi(v)\right) + \sin^2 \vartheta \, w^t A (A^{-1} - \psi(v) B^{-1}) A w, \tag{5.26}$$

and (3.17) turns into

$$\|s\|_{B^{-1}}^2 = \sin^2 \vartheta \, w^t A (A^{-1} - \psi(v) B^{-1}) B (A^{-1} - \bar\lambda^{-1} B^{-1}) A w. \tag{5.27}$$

To this, one must apply the Cauchy-Schwarz inequality for the B^{-1}-inner product. Note that the quantities involved are again from two 'folded' pencils as in (5.24).

By noting that $A\bar v \perp_{B^{-1}} Aw \Rightarrow \bar v \perp Aw$, (5.21) becomes a direct extension of Theorem 3.12.

The proof of (5.22) is completely analogous to the one of Theorem 3.14 and makes use of (5.26) and (5.27).

Proceeding as in the proof of Theorem 3.16, one obtains as generalization of (3.25)

$$\nabla^2 \psi(v) = \frac{2}{v^t A B^{-1} A v} A \left\{ \left(A^{-1} - \psi(v) B^{-1}\right) \right. \\ \left. -2 \frac{\left(A^{-1} - \psi(v) B^{-1}\right) A v v^t A B^{-1} + B^{-1} A v v^t A \left(A^{-1} - \psi(v) B^{-1}\right)}{(v^t A B^{-1} A v)} \right\} A.$$

As (5.13) says that $v^t A \left(A^{-1} - \psi(v) B^{-1}\right) A v = 0$ one has (5.23). □

Even though it looks unusual, the metric induced by the inner product with B^{-1} in (5.20) is natural and consistent with the proposed normalization (5.14). In [9], similar metrics are used in an analysis of shift-invert Lanczos.

At last, we comment on the interesting observation that in both standard and generalized case, ψ is a quotient of Rayleigh and 'folded' ([16, 'Method 2'][36]) Rayleigh quotient. This is clear in the standard case

$$\psi(v) = \tfrac{v^t A v}{v^t v} \Big/ \tfrac{v^t A^2 v}{v^t v} \tag{5.28}$$

but equally true in the generalized one:

$$\psi(v) = \tfrac{v^t A v}{v^t B v} \Big/ \tfrac{v^t A B^{-1} A v}{v^t B v}. \tag{5.29}$$

When v is an eigenvector, one has as expected $\psi(v) = 1/\rho(v)$. (Note that A is assumed to be nonsingular.) Otherwise, the general relationship can be derived from (5.29) and $Av = \rho B v + r(v)$, $v \perp r(v)$, to yield

$$\psi(v) = \frac{\rho(v) \|Bv\|_{B^{-1}}^2}{\rho^2(v) \|Bv\|_{B^{-1}}^2 + \|r(v)\|_{B^{-1}}^2} = \frac{\rho(v)}{\rho^2(v) + \|r(v)\|_{B^{-1}}^2 / \|Bv\|_{B^{-1}}^2}. \tag{5.30}$$

Thus, $\|r(v)\|_{B^{-1}}^2$ measures how much ψ deviates from ρ^{-1}, in the direction towards zero. It is also this term that makes all the difference for indefinite A, compared to the simply reversed Rayleigh quotient from (2.7).

6. Conclusions and perspective. This paper investigates harmonic Ritz values in their role as approximants to interior eigenvalues of a real symmetric matrix. Instead of the standard derivation from a Petrov Galerkin condition, we follow a functional-based approach and consider the reversed harmonic Rayleigh quotient ψ.

Guided by the gradient $\nabla\psi$, we derived a new type of residual s. We showed that the theory for ψ and s. parallels in remarkable ways the one of the standard Rayleigh quotient. Useful features including minimal residual and Weinstein-type bounds and expressions for backward error Hessian matrix have been established.

As ψ remains bounded even for an indefinite nonsingular matrix A, it lends itself to the computation of interior eigenvalues. A first immediate application is a 'Rayleigh-quotient' like iteration. Of arguably even greater practical relevance is its use in an optimization method such as (nonlinear) Preconditioned Conjugate Gradients [3, 20, 24]. LOBPCG [14] can also be generalized to this scenario. Instead of computing the smallest/largest eigenvalue of A by minimizing/maximizing the Rayleigh quotient, one can compute interior eigenvalues of A with PCG and LOBPCG as the minimum/maximum of ψ.

Thus, ψ can be used as an alternative to the 'folded' Rayleigh quotient [16, 'Method 2'][36] which, for example, is an important tool for calculating the photoluminescence of nano-structures [34, 35, 36].

The advantage of ψ is its connection to the inverse. An eigenvalue that used to be to the left (right) of zero, or the chosen shift, gets mapped towards $-\infty$ ($+\infty$). As in inverse iteration, this facilitates the selection of eigenpairs by their location respective to a point of interest. Moreover, one avoids eigenvalues from the left and right being folded together and into each other, a danger commonly present when squaring the matrix in the folded approach.

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