VARIATIONS ON HARMONIC RAYLEIGH–RITZ FOR STANDARD AND GENERALIZED EIGENPROBLEMS

MICHIEL E. HOCHSTENBACH*

Abstract. We present several variations on the harmonic Rayleigh–Ritz method. First, we introduce a relative harmonic approach for the standard, generalized, and polynomial eigenproblem. Second, a harmonic extraction method is studied for rightmost eigenvalues of generalized eigenvalue problems. Third, we propose harmonic extraction methods for large eigenvalues of generalized and polynomial eigenproblems, where we also discuss avoidance of infinite eigenvalues when the finite eigenvalues are of interest. We give an oversight of the different methods with their relations and several typical numerical examples.

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1. Introduction. The harmonic Rayleigh–Ritz subspace extraction, mainly due to early work by Morgan [11] and its formal introduction by Paige, Parlett, and Van der Vorst [12] is a very helpful technique to approximate eigenvalues in the interior of the spectrum.

First consider the standard eigenvalue problem $Ax = \lambda x$ for a given large, sparse $n \times n$ matrix A. Let $\mathcal{U} \subset \mathbb{C}^n$ be a k-dimensional search space. The standard Rayleigh–Ritz approach to extract approximate eigenpairs $(\theta, u) \approx (\lambda, x)$ where $u \in \mathcal{U}$ is to impose the Galerkin condition

$$Au - \theta u \perp \mathcal{U}.$$

If we write $u = Uc$, $c \in \mathbb{C}^k$, this leads to the projected eigenvalue problem $U^*AUc = \theta c$. It is well known that this extraction is in practice often favorable for exterior, but unfavorable for interior eigenvalues, see for instance [17] and also Section 4.

Interior eigenvalues λ close to a target τ are exterior eigenvalues of $(A - \tau I)^{-1}$. This suggests to consider to impose a Galerkin condition on this spectrally transformed problem $(A - \tau I)^{-1}x = (\lambda - \tau)^{-1}x$:

$$(A - \tau I)^{-1}u - (\theta - \tau)^{-1}u \perp \mathcal{V},$$

where $\mathcal{V}$ is a certain test space and I is the identity matrix. To avoid working with the inverse of a large sparse matrix, which is in practice often expensive or even infeasible, we choose $\mathcal{V} = (A - \tau I)^*(A - \tau I)\,\mathcal{U}$. The harmonic Ritz extraction is then defined by

$$U^*(A - \tau I)^*(A - \tau I)\,u = (\theta - \tau)\,U^*(A - \tau I)^*u.$$

With the notation $\xi = \theta - \tau$ and $u = Uc$, we are interested in the eigenpairs (ξ, c) of the projected generalized eigenproblem

$$U^*(A - \tau I)^*(A - \tau I)Uc = \xi\,U^*(A - \tau I)^*Uc, \qquad \xi = \theta - \tau, \tag{1.1}$$

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Department of Mathematics, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106-7058, USA, hochsten@case.edu, www.case.edu/artsci/math/hochstenbach. The research of this author was supported in part by NSF grant DMS-0405387.

for which $|\xi|$ is minimal. In [6], the term *(harmonic) factor* was coined for ξ. In [17] it was shown that an eigenpair (λ, x) has the desirable property that it is also a harmonic Ritz pair with respect to the search space span(x). Moreover, for a harmonic Ritz vector u with factor ξ we have (left-multiply (1.1) by c^* and use the Cauchy–Schwarz inequality)

$$\|Au - \tau u\| \leq |\xi|.$$

This provides us with a bound on the residual, in contrast to an approximate eigenpair derived by the standard Ritz extraction.

A generalization of the harmonic extraction for the generalized eigenvalue problem $Ax = \lambda Bx$ was presented by Stewart [17]; see also Fokkema, Sleijpen, and Van der Vorst [3]. We start from the spectrally transformed problem

$$(A - \tau B)^{-1} Bx = (\lambda - \tau)^{-1} x$$

which maps the eigenvalues close to τ to the exterior of the spectrum. Choosing the search space $\mathcal{V} = (A - \tau B)^*(A - \tau B)\,\mathcal{U}$ in the associated Galerkin condition

$$(A - \tau B)^{-1} Bu - (\theta - \tau)^{-1} u \perp \mathcal{V},$$

gives

$$U^*(A - \tau B)^*(A - \tau B)Uc = \xi\, U^*(A - \tau B)^* BUc, \qquad \xi = \theta - \tau. \tag{1.2}$$

Any eigenpair (ξ, c) yields a harmonic Ritz pair (θ, Uc), $\theta = \xi + \tau$, with

$$\|Au - \tau Bu\| \leq |\xi|\, \|Bu\|. \tag{1.3}$$

A "Saad-like" result on harmonic vectors for the standard eigenproblem was presented by Chen and Jia [2]. We now (straightforwardly) generalize their result for the generalized eigenproblem.

Let u be a harmonic Ritz vector, $[u\ V]$ be an orthonormal basis for $\mathcal{U}$, and $[u\ V\ W]$ be an orthonormal basis for $\mathbb{C}^n$. Define

$$F = [u\ V]^*(A - \tau B)^*(A - \tau B)[u\ V] \quad \text{and} \quad E = [u\ V]^*(A - \tau B)^* B\,[u\ V];$$

we will assume that E is invertible. Denote by e_1 the first column of the identity matrix. Since

$$(A - \tau B)^*(A - \tau B)\, u - \xi\, (A - \tau B)^* B\, u \perp \mathcal{U},$$

we have $E^{-1} F e_1 = \xi e_1$, so $E^{-1} F$ is of the form

$$E^{-1} F = \begin{bmatrix} \xi & g^* \\ 0 & G \end{bmatrix}. \tag{1.4}$$

Since the eigenvalues of $E^{-1} F$ are the harmonic factors, the eigenvalues of G are the harmonic factors with the exception of ξ.

Theorem 1.1. *Let u be a harmonic Ritz vector with factor ξ for $Ax = \lambda Bx$ with respect to the search space $\mathcal{U}$ and let E be invertible. Then*

$$\sin(u, x) \leq \sin(\mathcal{U}, x) \sqrt{1 + \frac{\gamma^2\, \|E^{-1}\|^2}{\delta^2}},$$

where

$$\gamma = |\tau|\, \|P_{\mathcal{U}}\,(A-\tau B)^*(A-\lambda B)(I-P_{\mathcal{U}})\|,$$
$$\delta = \mathrm{sep}(\lambda-\tau,\, G) := \sigma_{\min}(G-(\lambda-\tau)I) \le \min_{\xi_j\neq\xi} |\xi_j-(\lambda-\tau)|,$$

$P_{\mathcal{U}}$ is the orthogonal projection onto $\mathcal{U}$, G is defined as in (1.4) *and the ξ_j range over the harmonic factors not equal to ξ.*

Proof. This is a generalization of [2] to the generalized eigenvalue problem, the proof is similar to that of Theorem 1.1 in Section 2.2. □

This theorem means that if the angle of the search space $\mathcal{U}$ and the eigenvector x tends to zero and if ξ is a simple factor, then there is a harmonic Ritz vector that converges to x.

The harmonic Ritz extraction was generalized for the polynomial eigenvalue problem

$$p(\lambda) = (\lambda^m A_m + \cdots + A_0)\, x = 0, \tag{1.5}$$

where $A_0, \ldots, A_m$ are real or complex $n \times n$ matrices, in [7] by two variants. First, for $\lambda \approx \tau$, the first order approximation

$$0 = p(\lambda)\, x \approx p(\tau)\, x + (\lambda-\tau)p'(\tau)\, x \tag{1.6}$$

gives the modified *approximate* eigenproblem

$$p(\tau)^{-1}p'(\tau)\, x \approx (\tau-\lambda)^{-1}x.$$

Choosing $\mathcal{V} = p(\tau)^*p(\tau)\,\mathcal{U}$ in the associated Galerkin condition

$$p(\tau)^{-1}p'(\tau)u - (\tau-\lambda)^{-1}u \perp \mathcal{V}$$

gives the linearized harmonic approach

$$U^*p(\tau)^*p(\tau)Uc = (\tau-\theta)U^*p(\tau)^*p'(\tau)Uc. \tag{1.7}$$

The linearized harmonic approach has the advantage that we can bound

$$\|p(\tau)u\| \le |\xi|\, \|p'(\tau)u\|, \qquad \xi = \theta-\tau, \tag{1.8}$$

but the disadvantage that an eigenpair is in general no linearized harmonic pair. The (non-linearized) harmonic approach, which includes the neglected terms in (1.6), is given by [7]

$$p(\theta)u \perp p(\tau)\,\mathcal{U}. \tag{1.9}$$

For the (non-linearized) harmonic approach the situation is exactly opposite compared to the linearized harmonic method: an exact eigenvector is a harmonic Ritz vector (with respect to the search space spanned by it), but there is no error bound on the residual norm similar to (1.8). Practically, the (non-linearized) harmonic approach, or a combination of the two techniques in different stages of the process, seems to work best in practice; see [7] for more details.

In this paper we propose several variants on harmonic Rayleigh–Ritz. In Section 2 we discuss the problem of finding interior eigenvalues that are closest to a target in a *relative* instead of absolute sense. Section 3 proposes an approach to find *rightmost* eigenvalues of the generalized eigenproblem. The harmonic Ritz method has always been advocated for interior eigenvalues. In Section 4 we show that a harmonic approach may also be useful to find *exterior* eigenvalues for the generalized and polynomial eigenproblem, also for the computation of finite eigenvalues in the presence of infinite eigenvalues. After discussing various details in Section 5, we finish with some numerical experiments and conclusions in Sections 6 and 7.

2. Relative harmonic extraction. The standard harmonic Rayleigh–Ritz extracts approximate eigenpairs $(\theta, u) \approx (\lambda, x)$ with $|\theta - \lambda|$ small, that is, of which the approximate eigenvalue θ is close to a target τ in an *absolute* sense. We may also be interested in the eigenvalues that are closest to a target in a *relative* sense. Thus, given a target τ, we want to find eigenvalues $\lambda \neq 0$ such that

$$\frac{|\lambda - \tau|}{|\lambda|} = |1 - \tau\lambda^{-1}|$$

is minimal. We will now develop methods to try to accomplish this for the standard, generalized, and polynomial eigenvalue problem in the next three subsections. As we see, the relative harmonic extraction for the standard eigenvalue problem in Section 2.1 is a special instance of the rational harmonic extraction [6].

2.1. The standard eigenvalue problem. For the standard eigenvalue problem $Ax = \lambda x$ we are interested in minimal eigenvalues (in absolute value sense) of

$$(I - \tau A^{-1})\, x = (1 - \tau\lambda^{-1})\, x,$$

whereby we assume that $\lambda \neq 0$, which is a natural hypothesis for a relative approach. As stated before, Galerkin conditions usually work favorably for exterior eigenvalues. Therefore, we consider a Galerkin condition on the inverted problem

$$(I - \tau A^{-1})^{-1} u - \xi^{-1} u \perp \mathcal{V}, \qquad \xi = 1 - \tau\theta^{-1}, \tag{2.1}$$

or, equivalently,

$$(A - \tau I)^{-1} A u - \xi^{-1} u \perp \mathcal{V}, \qquad \xi = 1 - \tau\theta^{-1},$$

for a certain test space $\mathcal{V}$. We want to take $\mathcal{V}$ such that we can avoid working with the inverse of a large (sparse) matrix. One may check that the choice $\mathcal{V} = (A - \tau I)^* \mathcal{U}$ leads to the standard Ritz–Galerkin condition

$$Au - \theta u \perp \mathcal{U},$$

with the correspondence $\xi = 1 - \tau\theta^{-1}$. The standard extraction may extract Ritz pairs (θ, u) with the smallest $|\xi| = |1 - \tau\theta^{-1}|$, but there is no bound on the residual norm, so that the approximate eigenvector may be of poor quality. With the choice $\mathcal{V} = (A - \tau I)^*(A - \tau I)\mathcal{U}$ we get

$$U^*(A - \tau I)^*(A - \tau I)\, u = \xi\, U^*(A - \tau I)^* A u, \qquad \xi = 1 - \tau\theta^{-1}. \tag{2.2}$$

A pair satisfying (2.2) satisfies

$$\|(A-\tau I)\,u\| \le |\xi|\,\|Au\|.$$

This means that if there is a pair (ξ, u) of (2.2) with a small $|\xi| = |1-\tau\theta^{-1}|$, the approximate eigenvalue θ is close to τ in a relative sense and the approximate eigenvector u has a small residual norm $\|Au-\tau u\|$, and hence also a small $\|Au-\theta u\|$. Moreover, if (λ, x) is an eigenpair, then it satisfies (2.2) with $\xi = 1-\tau\lambda^{-1}$ for any search space $\mathcal{U}$. These two facts form a justification of the approach to select the pair(s) of (2.2) with the smallest $|\xi|$.

We note that this relative harmonic extraction is a special instance of the rational harmonic extraction [6] if in the rational eigenproblem

$$q(A)\,x = (q(\lambda)/r(\lambda))\,r(A)\,x$$

we choose $q(z) = z-\tau$ and $r(z) = z$. Yet another equivalent way to write (2.2) and (2.1) is

$$(A-\tau I)\,u - \xi\,Au \perp (A-\tau I)\,\mathcal{U}, \qquad \xi = 1-\tau\theta^{-1},$$

or

$$(A-\theta I)\,u \perp (A-\tau I)\,\mathcal{U}, \qquad \theta = \frac{\tau}{1-\xi} \tag{2.3}$$

(with the convention that θ is infinite if $\xi = 1$). In the last Galerkin condition we recognize the (standard) harmonic Ritz extraction, but with a special ordering on the harmonic Ritz pairs (θ, u) with respect to increasing $|\xi| = |1-\tau\theta^{-1}|$ values. Therefore, the relative harmonic vectors are the same as the (standard) harmonic vectors, but in the relative harmonic extraction we select the harmonic vector of which the harmonic Ritz value is closest to τ in a *relative* instead of absolute sense.

2.2. The generalized eigenvalue problem. Recall that for the generalized eigenproblem $Ax = \lambda Bx$, the usual harmonic approach is given by (1.2) with associated residual bound (1.3). For the relative harmonic extraction for the generalized eigenvalue problem with target τ our starting point is

$$(A-\tau B)\,x = (\lambda-\tau)Bx = (1-\tau\lambda^{-1})Ax.$$

Since we are interested in λ with small $|1-\tau\lambda^{-1}|$, we consider the inverted problem $(A-\tau B)^{-1}Ax = (1-\tau\lambda^{-1})^{-1}x$. With the Galerkin condition

$$(A-\tau B)^{-1}Au - (1-\tau\theta^{-1})^{-1}u \perp (A-\tau B)^*(A-\tau B)\,\mathcal{U}$$

we get a straightforward generalization of (2.2):

$$U^*(A-\tau B)^*(A-\tau B)\,Uc = \xi\,U^*(A-\tau B)^*AUc, \qquad \xi = 1-\tau\theta^{-1}. \tag{2.4}$$

A backtransformed pair (ξ, Uc) satisfies

$$\|(A-\tau B)u\| \le |\xi|\,\|Au\|. \tag{2.5}$$

If we select a pair (ξ, u) with a small $|\xi|$, we know that it is a good approximate eigenpair and that $\theta \approx \tau$ in a relative sense. Note that for the "extreme" case $\tau = 0$, the extraction (2.4) is meaningless since every vector satisfies this equation with $\xi = 1$.

As in (2.3), we have that the relative harmonic method for the generalized eigenproblem is equivalent with

$$(A - \theta B)\, u \perp (A - \tau B)\,\mathcal{U}, \qquad \theta = \frac{\tau}{1-\xi}, \qquad \xi = 1 - \tau\theta^{-1};$$

again, we conclude that the relative harmonic extraction for the generalized eigenvalue problem gives the same approximate vectors as the harmonic extraction, but in the relative harmonic extraction we select the harmonic vector of which the harmonic Ritz value is closest to τ in a *relative* sense.

Another connection between the relative and standard harmonic methods is the following. If $\tau \neq 0$, then selecting the pair with the smallest $|\xi|$ from

$$(A - \tau B) - \xi\, Au \perp (A - \tau B)\,\mathcal{U},$$

as is done in the relative harmonic approach, is equivalent to selecting the pair with the smallest $|\xi\,\tau^{-1}|$ from

$$(\tau^{-1}A - B) - \xi\,\tau^{-1}\, Au \perp (\tau^{-1}A - B)\,\mathcal{U}.$$

We may recognize this Galerkin condition as the standard harmonic approach on the modified problem $Bx = \mu\, Ax$ with target τ^{-1}.

Inspired by a result by Chen and Jia [2], we have the following theorem; cf. also Theorem 1.1. Let (θ, u) be a relative harmonic pair with factor ξ $(= 1 - \tau\theta^{-1})$, $[u\ V]$ be an orthonormal basis for $\mathcal{U}$, and $[u\ V\ W]$ be an orthonormal basis for $\mathbb{C}^n$. We first write

$$\widetilde{F} = [u\ V]^*(A - \tau B)^*(A - \tau B)[u\ V] \quad \text{and} \quad \widetilde{E} = [u\ V]^*(A - \tau B)^* A\,[u\ V],$$

and we will assume that $\widetilde{E}$ is invertible. Since for the relative harmonic extraction (cf. (2.4))

$$(A - \tau B)^*(A - \tau B)\, u - \xi\,(A - \tau B)^* A\, u \perp \mathcal{U},$$

we have $\widetilde{E}^{-1}\widetilde{F}e_1 = \xi e_1$, so $\widetilde{E}^{-1}\widetilde{F}$ is of the form

$$\widetilde{E}^{-1}\widetilde{F} = \begin{bmatrix} \xi & \widetilde{g}^* \\ 0 & \widetilde{G} \end{bmatrix}. \tag{2.6}$$

Since the eigenvalues of $\widetilde{E}^{-1}\widetilde{F}$ are the relative harmonic factors, the eigenvalues of $\widetilde{G}$ are the relative harmonic factors with the exception of ξ.

THEOREM 2.1. *Let u be a relative harmonic Ritz vector with factor ξ, λ be a nonzero eigenvalue and $\widetilde{E}$ be invertible. Then*

$$\sin(u, x) \le \sin(\mathcal{U}, x)\sqrt{1 + \frac{\widetilde{\gamma}^2\, \|\widetilde{E}^{-1}\|^2}{\widetilde{\delta}^2}},$$

where

$$\begin{aligned}\widetilde{\gamma} &= |\tau|\, \|P_{\mathcal{U}}\,(A-\tau B)^*(\lambda^{-1}A - B)(I-P_{\mathcal{U}})\|,\\ \widetilde{\delta} &= \operatorname{sep}(1-\tau\lambda^{-1},\, \widetilde{G}) := \sigma_{\min}(\widetilde{G} - (1-\tau\lambda^{-1})I) \le \min_{\xi_j\ne\xi} |\xi_j - (1-\tau\lambda^{-1})|,\end{aligned}$$

$P_{\mathcal{U}}$ is the orthogonal projection onto $\mathcal{U}$, $\widetilde{G}$ is defined as in (2.6)*, and the ξ_j range over the relative harmonic factors not equal to ξ.*

Proof. Introduce a new variable $z = [z_1^T\ z_2^T\ z_3^T]^T = [u\ V\ W]^* x$. From $(A-\tau B)\,x = (1-\tau\lambda^{-1})Ax$ we get $(A-\tau B)^*(A-\tau B)\,x = (1-\tau\lambda^{-1})(A-\tau B)^*Ax$ and

$$\begin{bmatrix} u^* \\ V^* \\ W^* \end{bmatrix} (A-\tau B)^*(A-\tau B)[u\ V\ W]\,z = (1-\tau\lambda^{-1}) \begin{bmatrix} u^* \\ V^* \\ W^* \end{bmatrix} (A-\tau B)^* A\,[u\ V\ W]\,z,$$

which we can write as

$$\begin{bmatrix} \widetilde{F} & F_1 \\ F_2 & F_3 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = (1-\tau\lambda^{-1}) \begin{bmatrix} \widetilde{E} & E_1 \\ E_2 & E_3 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix},$$

where $F_1 = [u\ V]^*(A-\tau B)^*(A-\tau B)W$ and $E_1 = [u\ V]^*(A-\tau B)^*AW$. Therefore we get

$$\widetilde{F} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + F_1 z_3 = (1-\tau\lambda^{-1})\, \widetilde{E} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + (1-\tau\lambda^{-1}) E_1 z_3$$

or

$$\left(\widetilde{E}^{-1}\widetilde{F} - (1-\tau\lambda^{-1})\,I\right) \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \widetilde{E}^{-1}\left((1-\tau\lambda^{-1})E_1 - F_1\right) z_3. \tag{2.7}$$

The right-hand side of (2.7) is bounded from above by

$$\|\widetilde{E}^{-1}\|\, \left\|[u\ V]^*(A-\tau B)^*((1-\tau\lambda^{-1})A - (A-\tau B))W\right\|\, \|z_3\| = \widetilde{\gamma}\ \|\widetilde{E}^{-1}\|\, \|z_3\|.$$

while the left-hand side of (2.7) can be bounded from below by

$$\begin{aligned}\left\| \begin{bmatrix} \xi - (1-\tau\lambda^{-1}) & \widetilde{g}^* \\ 0 & \widetilde{G} - (1-\tau\lambda^{-1})I \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \right\| &\ge \|(\widetilde{G} - (1-\tau\lambda^{-1})\,I)\,z_2\| \\ &\ge \operatorname{sep}(1-\tau\lambda^{-1}, \widetilde{G})\, \|z_2\|.\end{aligned}$$

Combining these two bounds, we have

$$\|z_2\| \le \frac{\widetilde{\gamma}\, \|\widetilde{E}^{-1}\|}{\widetilde{\delta}}\, \|z_3\|$$

Since $\sin^2(\mathcal{U}, x) = \|W^*x\|^2 = \|z_3\|^2$ and $\sin^2(x,u) = \|[V\ W]^*x\|^2 = \|z_2\|^2 + \|z_3\|^2$, the result now follows. □

Since $1-\tau\lambda^{-1}$ can be seen as the (relative harmonic) factor corresponding to the eigenvector x, $\widetilde{\delta}$ is less or equal to the minimum distance between the set of the (relative harmonic) factors ξ_j of the relative harmonic vectors (excluding ξ) and the factor of x. Moreover, $\widetilde{\delta}$ is not zero if ξ is a simple (relative harmonic) factor.

2.3. The polynomial eigenvalue problem. Now let us try to formulate a relative harmonic extraction for the polynomial eigenproblem (1.5). We use the first order Taylor expansions (cf. [7])

$$\begin{aligned} p(\tau)\,x &= (\tau-\lambda)p'(\eta_1)\,x, \quad \eta_1 \in [\tau,\lambda], \\ p(0)\,x &= -\,\lambda\,p'(\eta_2)\,x, \quad \eta_2 \in [0,\lambda], \end{aligned}$$

by which we mean that η_1 is on the line piece $\eta(t) = \lambda + t\,(\tau-\lambda)$, $t \in [0,1]$, from λ to τ and, similarly, η_2 is located between 0 and λ. If $\tau \approx 0$, then $\eta_1 \approx \eta_2$ which inspires us to consider the approximate eigenproblem

$$p(\tau)^{-1}p(0)\,x \approx (1-\tau\lambda^{-1})^{-1}\,x.$$

Therefore, we define the relative harmonic Ritz extraction for the polynomial eigenvalue problem by the Galerkin condition

$$p(\tau)\,u - \xi\,p(0)\,u \perp p(\tau)\,\mathcal{U}$$

or, equivalently with $u = Uc$,

$$U^*p(\tau)^*p(\tau)Uc = \xi\,U^*p(\tau)^*p(0)Uc. \tag{2.8}$$

Note that for the generalized eigenproblem ($p(\tau) = A - \tau B$) this approach reduces to (2.4). A difference with the method described in the previous subsection is formed by the fact that the approach for the polynomial eigenproblem is suitable only for small τ; on the other hand, this may be exactly the situation in which we are particularly interested in relative approximations.

A pair $(\xi, u) = (\xi, Uc)$ solving this projected eigenproblem satisfies (left-multiply by c^* and using Cauchy–Schwarz)

$$|\lambda-\tau|\,\|p'(\eta_1)\| = \|p(\tau)u\| \le |\xi|\,\|p(0)\,u\| = |\xi|\,|\lambda|\,\|p'(\eta_2)\|;$$

therefore, we are interested in the pair(s) solving (2.8) with the smallest $|\xi|$. However, an exact eigenpair is generally not a solution to (2.8), so we expect more modest results; see the numerical experiments. We note that having determined an approximate eigenvector, we can get an approximate eigenvalue by taking a Rayleigh quotient, or one of the alternatives presented in [8].

An alternative to (2.8), inspired by the previous subsection, would be to use the harmonic extraction (1.9) for the polynomial eigenproblem and take the approximate vector of which the value θ is *relatively* closest to the target. A potential problem with this approach is that for an approximate vector u the requirement (1.9) defines m possible values θ, where m is the degree of p; in general, only one of these is a sensible approximate eigenvalue.

3. The rightmost eigenvalues. In many applications, for instance stability problems, it is important to detect the rightmost eigenvalue(s). We first briefly recall relevant results from [6] for the standard eigenproblem before we generalize these to the generalized eigenproblem.

3.1. The standard eigenvalue problem. Suppose that A is an (almost) stable matrix, that is, the eigenvalues of A are (almost) located in the left-half plane; we are interested in finding the rightmost eigenpair. In [6] the starting point was the fact that the one-level curve of generalized Cayley transforms of the form

$$c(z) = \frac{z+\overline{\tau}}{z-\tau} \quad \text{or} \quad c(z) = \frac{z+\overline{\tau_1}}{z-\tau_1}\,\frac{z+\overline{\tau_2}}{z-\tau_2}, \quad \text{etc.},$$

where τ, τ_1, and τ_2 lie in the right-half plane, is exactly the imaginary axis. With the stability assumption on A, we know that the sought eigenvalues are the exterior eigenvalues of $c(A)$; a suitable test space ensures that we can avoid matrix inversion.

3.2. The generalized eigenvalue problem. We generalize this idea to the generalized eigenproblem. Suppose that the eigenvalues of the pencil (A, B) are (almost) in the left-half plane, then, with $\mathrm{Re}(\tau) > 0$, the rightmost eigenvalues are exterior eigenvalues of

$$(A-\tau B)^{-1}(A+\overline{\tau}B)x = \frac{\lambda+\overline{\tau}}{\lambda-\tau}\,x.$$

The associated Galerkin condition

$$(A-\tau B)^{-1}(A+\overline{\tau}B)Uc - \xi^{-1}\,Uc \perp (A-\tau B)^*(A-\tau B)\,\mathcal{U}$$

gives the extraction process

$$U^*(A-\tau B)^*(A-\tau B)Uc = \xi\, U^*(A-\tau B)^*(A+\overline{\tau}B)Uc. \tag{3.1}$$

Here we have the one-one correspondence

$$\theta = \frac{\tau+\overline{\tau}\xi}{1-\xi}, \qquad \xi = \frac{\theta-\tau}{\theta+\overline{\tau}}.$$

The solutions (ξ, u), $u = Uc$, to (3.1) satisfy

$$\|(A-\tau B)u\| \le |\xi|\, \|(A+\overline{\tau}B)u\|.$$

If we select the pair (ξ, Uc) with the smallest $|\xi|$, we hope that this approach tends to select eigenpairs (λ, x) for which

$$|\lambda-\tau|\,\|Bx\| = \|(A-\tau B)x\| \ll \|(A+\overline{\tau}B)x\| = |\lambda+\overline{\tau}|\,\|Bx\|.$$

Assuming that $Bx \ne 0$ ($Bx = 0$ corresponds to a infinite or even undefined eigenvalue), our eigenvalue will then have a small $|\lambda-\tau|/|\lambda+\overline{\tau}|$ ratio.

This extraction for the rightmost eigenvalue also has a close connection with the (standard) harmonic extraction: (3.1) is equivalent to

$$(A-\theta B)\,u \perp (A-\tau B)\,\mathcal{U}, \qquad \theta = \frac{\tau+\overline{\tau}\xi}{1-\xi}, \qquad \xi = \frac{\theta-\tau}{\theta+\overline{\tau}}.$$

Therefore, this extraction process selects the harmonic Ritz pair (θ, u) with the smallest $|\xi| = \frac{|\theta-\tau|}{|\theta+\overline{\tau}|}$ value. Unfortunately, a product of two or more generalized Cayley transforms as may be used for the standard eigenvalue problem (see [6]) seems impractical since factors of the form $A-\sigma B$ and $A-\tau B$ do not commute in general.

3.3. The polynomial eigenvalue problem. For the polynomial eigenvalue problem (1.5), we may—inspired by the connection with the standard harmonic extraction in the last subsection—use the harmonic extraction (1.9) and extract the pair with the smallest $|\theta - \tau|/|\theta + \overline{\tau}|$ value. However, as in Section 2.3, this has the difficulty that not all values θ are sensible eigenvalue approximations.

4. Harmonic extraction for large eigenvalues.

As also stated in the introduction, the standard extraction has the reputation of being favorable for large eigenvalues. For the generalized Hermitian/positive definite eigenvalue problem

$$Ax = \lambda Bx, \quad A^* = A, \ B^* = B, \ B > 0,$$

this can be substantiated. Let u be an approximation to the eigenvector x. The eigenvectors $x_1, \ldots, x_n$ of this problem can be chosen B-orthonormal, and we can write

$$u = \sum_{j=1}^{n} \gamma_j \, x_j.$$

Assume without loss of generality that $u^*Bu = 1$. The Rayleigh quotient ρ of u is

$$\rho = \frac{u^*Au}{u^*Bu} = \sum_{j=1}^{n} |\gamma_j|^2 \, \lambda_j.$$

Therefore, we know that

- if the exterior eigenvalues are not clustered: $\lambda_1 < \lambda_2 \le \cdots \le \lambda_{n-1} < \lambda_n$,
- and if ρ approaches one of the exterior eigenvalues, $\rho \approx \lambda_1$ or $\rho \approx \lambda_n$,

then u must be close to x_1 or x_n, respectively.

However, for many other eigenvalue problems, for instance non-Hermitian problems, there is limited theoretical evidence why the standard extraction would be favorable for exterior eigenvalues; examples can be constructed where the standard extraction encounters difficulties [16]. An exception is a result by Van den Eshof [18], that shows that in some circumstances the standard Rayleigh–Ritz extraction is asymptotically (that is, when the angle of the search space with the eigenvector is small enough) is safe to use.

In this section, we are interested in extraction methods to approximate the largest eigenpairs for the generalized and polynomial eigenproblem; these methods have a different theoretical basis.

4.1. Harmonic extraction for large eigenvalues of the generalized eigenvalue problem. If we are interested in exterior eigenvalues of $Ax = \lambda Bx$, we can think of the line at infinity in the complex plane as the target. The main observation is that we may instead take the target $\tau = 0$ for the modified eigenproblem

$$Bx = \mu Ax, \quad \mu = 1/\lambda.$$

When we apply the (standard) harmonic Ritz approach on this eigenproblem (see (1.2)), we are interested in eigenpairs (ξ, c) of

$$U^*B^*BUc = \xi \, U^*B^*AUc, \qquad \xi = \theta^{-1}, \tag{4.1}$$

corresponding to small $|\xi|$. If $u = Uc$ is such a vector corresponding to a small $|\xi|$, then

$$\|Bu\| \le |\xi|\, \|Au\|;$$

this means that if u is a good approximation to an eigenvector, then for the corresponding eigenvalue we have

$$|\lambda| \approx \|Au\|/\|Bu\| \lesssim |\xi|^{-1}.$$

This, combined with the fact that if $(\lambda, x) = (\lambda, Uc)$ is an eigenpair, (λ^{-1}, x) is also a solution of (4.1), gives confidence that the harmonic extraction (4.1) for large eigenvalues is asymptotically safe. We note that (4.1) is equivalent to the Petrov–Galerkin condition

$$AUc - \xi^{-1} BUc \perp B\mathcal{U}.$$

This extraction is sometimes also preferred over the standard extraction $U^*AUc = \theta\, U^*BUc$ since the orthogonality condition $r = Au - \theta Bu \perp Bu$ ensures that the residual r is minimal over all choices of θ. See [4] for early work on similar Galerkin conditions.

4.2. Harmonic extraction for large eigenvalues of the polynomial eigenvalue problem. Now we move to the polynomial eigenvalue problem (1.5). As mentioned in the introduction, [7] proposed two different harmonic approaches for this problem: the linearized harmonic approach (1.7) and the (non-linearized) harmonic approach (1.9).

Similar to the situation in the generalized eigenproblem in the previous subsection we will use the fact that large eigenvalues of (1.5) are small eigenvalues of the modified problem with polynomial $\widetilde{p}(\mu) := \mu^m p(\mu^{-1})$:

$$\widetilde{p}(\mu)\, x = (A_m + \cdots + \mu^m A_0)\, x = 0. \tag{4.2}$$

The linearized harmonic approach (1.7) applied to this problem with target $\tau = 0$ is $\widetilde{p}(0)\, u - \xi\, \widetilde{p}'(0) u \perp \widetilde{p}(0)\, \mathcal{U}$ or in other words

$$A_m u - \xi\, A_{m-1} u \perp A_m \mathcal{U}. \tag{4.3}$$

The (non-linearized) harmonic approach (1.9) applied to this problem renders $\widetilde{p}(1/\theta) \perp \widetilde{p}(0)\, \mathcal{U}$ or

$$p(\theta)\, u \perp A_m \mathcal{U} \tag{4.4}$$

One may check that for the generalized eigenvalue problem both reduce to (4.1). The linearized harmonic approach has the bound

$$\|A_m u\| \le |\xi|\, \|A_{m-1} u\|.$$

If x is an eigenvector corresponding to a large eigenvalue, then heuristically we expect

$$0 = p(\lambda)\, x \approx \lambda^m A_m x + \lambda^{m-1} A_{m-1} x,$$

which implies that the ratio $\|A_m x\|/\|A_{m-1} x\| \approx |\lambda|^{-1}$ should be small. However, an exact eigenvector will not satisfy (4.3) in general. Since an exact eigenpair does satisfy (4.4), we expect that this approach will be often be superior to (4.3), cf. [7].

4.3. Avoiding infinite eigenvalues. For many applications that lead to a generalized eigenproblem, one is interested in the largest or rightmost *finite* eigenvalue; see for instance [13]. If a generalized eigenproblem also has infinite eigenvalues, these are often an enormous hinderance for convergence. In some applications, the null space of B is low-dimensional and explicitly known and one may try to “deflate” this space. However, in other applications the null space is either unknown or large, so that deflation becomes unattractive. We now show that the harmonic extraction may also be practical for this situation.

Let (A, B) be a pencil where B is singular. Suppose that we are interested in the largest or rightmost finite eigenvalue(s) and that we have a (very rough) estimation τ for the relevant values. Then we may also try to compute the eigenvalues of the modified problem $Bx = \mu Ax$ that are close, but not equal to zero. In other words, with a target $\tau^{-1} \approx 0$, we would like to compute eigenvectors x such that

$$\|(B - \tau^{-1}A)\, x\| \ll \|Bx\|.$$

Inspired by Section 3, we may try to accomplish this by imposing the Galerkin condition

$$U^*(\tau^{-1}A - B)^*(\tau^{-1}A - B)\, u = \xi\, U^*(\tau^{-1}A - B)^*Bu.$$

and selecting the pair(s) corresponding to the smallest $|\xi|$. We recognize the equivalent

$$(\tau^{-1}A - B)\, u - \xi\, Bu \perp (\tau^{-1}A - B)\,\mathcal{U}$$

as the relative harmonic approach applied to the modified problem $Bx = \mu Ax$ with target $\tau^{-1} \approx 0$; or the equivalent

$$(A - \tau B)\, u - \tau\, \xi\, Bu \perp (A - \tau B)\,\mathcal{U}$$

as the standard harmonic Ritz extraction with target τ, bearing in mind that selecting the smallest $|\tau\, \xi|$ is equivalent to selecting the smallest $|\xi|$. Therefore, the harmonic extraction is a valuable to avoid infinite eigenvalues.

For the polynomial eigenvalue problem (1.5), we would like to find eigenvectors x with

$$\|\widetilde{p}(\tau^{-1})x\| \ll \|\widetilde{p}(0)x\|.$$

This suggests to select the smallest pairs (ξ, u) of

$$U^*\widetilde{p}(\tau^{-1})^*\widetilde{p}(\tau^{-1})\, u = \xi\, U^*\widetilde{p}(\tau^{-1})^*\widetilde{p}(0)\, u.$$

One may check that this is equivalent to taking the smallest pairs of

$$p(\tau)\, u - \xi\, A_m\, u \perp p(\tau)\,\mathcal{U}.$$

This may be recognized as an approximation to (1.7) for large τ. Another option is to (as for the generalized eigenproblem above) to use the standard harmonic extraction (1.9) and select the Ritz pair closest to the target τ.

5. Various issues.

5.1. A unifying framework for the generalized eigenproblem. All proposed generalization of the harmonic Rayleigh–Ritz methods for the generalized eigenproblem fit in the framework provided by the Galerkin condition

$$(\alpha A - \beta B)\, u - \xi\, (\gamma A - \delta B)\, u \perp (\alpha A - \beta B)\,\mathcal{U},$$

for certain $\alpha, \beta, \gamma, \delta$, where

$$\xi = \frac{\alpha\theta - \beta}{\gamma\theta - \delta}, \qquad \theta = \frac{\delta\xi - \beta}{\gamma\xi - \alpha}.$$

In Table 5.1 we list the different harmonic approaches with the corresponding choice for α, β, γ, and δ.

TABLE 5.1: A framework for the approaches and their use for the generalized eigenproblem.

Choice α, β	Choice γ, δ	Use
$\beta/\alpha = \tau/1$	$\delta/\gamma = \ \ 1/0$	Harmonic Rayleigh–Ritz
$\beta/\alpha = \tau/1$	$\delta/\gamma = \ \ 0/1$	Relative harmonic Rayleigh–Ritz
$\beta/\alpha = \tau/1$	$\delta/\gamma = -\overline{\tau}/1$	Rightmost eigenvalues
$\beta/\alpha = 1/0$	$\delta/\gamma = \ \ 0/1$	Largest eigenvalues

5.2. A summary. We now give a summary of most extraction methods presented in [6], [7], and this paper in Tables 5.2, 5.3, and 5.4. In all cases, we are interested in the pair(s) (ξ, u) with the smallest $|\xi|$, or in the pair(s) (θ, u) with θ closest to a target τ.

TABLE 5.2: A summary of extraction methods for the standard eigenvalue problem $Ax = \lambda x$.

Galerkin condition		Use
$(A - \tau I)\, u - \xi u$	$\perp \mathcal{U}$	Standard Rayleigh–Ritz
$(A - \tau I)\, u - \xi u$	$\perp (A - \tau I)\,\mathcal{U}$	Harmonic Rayleigh–Ritz
$(A - \tau I)\, u - \xi\, Au$	$\perp (A - \tau I)\,\mathcal{U}$	Relative harmonic Rayleigh–Ritz
$(A - \tau I)\, u - \xi\, (A + \overline{\tau} I)\, u$	$\perp (A - \tau I)\,\mathcal{U}$	Rightmost eigenvalue [6]

TABLE 5.3: A summary of extraction methods for the generalized eigenvalue problem $Ax = \lambda Bx$.

Galerkin condition		Use
$(A - \tau B)\, u - \xi\, Bu$	$\perp \mathcal{U}$	Standard Rayleigh–Ritz
$(A - \tau B)\, u - \xi\, Bu$	$\perp (A - \tau B)\,\mathcal{U}$	Harmonic Rayleigh–Ritz
		Largest eigenvalue in presence of ∞ eigenvalues
$(A - \tau B)\, u - \xi\, Au$	$\perp (A - \tau B)\,\mathcal{U}$	Relative harmonic Rayleigh–Ritz
$(A - \tau B)\, u - \xi\, (A + \overline{\tau} B)\, u$	$\perp (A - \tau B)\,\mathcal{U}$	Rightmost eigenvalue
$Bu - \xi\, Au$	$\perp B\mathcal{U}$	Largest eigenvalue

5.3. Refined extraction for large eigenvalues. If we are interested in approximating the largest eigenpairs of $p(\lambda)\, x = 0$ from a search space $\mathcal{U}$, we can also try a refined extraction. The refined Rayleigh–Ritz extraction was advocated for the standard eigenvalue problem by Jia [9]. Given τ, which is typically either a Ritz value or a fixed target, this approach determines an approximate eigenvector by minimizing the residual over the search space:

$$u = \underset{\widetilde{u} \in \mathcal{U},\ \|\widetilde{u}\| = 1}{\operatorname{argmin}} \ \|(A - \tau I)\, \widetilde{u}\|.$$

TABLE 5.4: A summary of extraction methods for the polynomial eigenproblem $(\lambda^m A_m + \cdots + A_0)x = 0$.

Galerkin condition		Use
$p(\theta)\, u$	$\perp \mathcal{U}$	Standard Rayleigh–Ritz
$p(\theta)\, u$	$\perp p(\tau)\mathcal{U}$	Harmonic Rayleigh–Ritz [7]
		Largest eigenvalue in presence of ∞ eigenvalues
$p(\tau)\, u - \xi\, p'(\tau)\, u$	$\perp p(\tau)\mathcal{U}$	Linearized harmonic Rayleigh–Ritz [7]
$p(\tau)\, u - \xi\, p(0)\, u$	$\perp p(\tau)\mathcal{U}$	Relative harmonic Rayleigh–Ritz
$p(\theta)\, u$	$\perp A_m\mathcal{U}$	Largest eigenvalue
$A_m u - \xi\, A_{m-1} u$	$\perp A_m\mathcal{U}$	Largest eigenvalue (linearized)
$p(\tau)\, u - \xi\, A_m\, u$	$\perp p(\tau)\mathcal{U}$	Largest eigenvalue in presence of ∞ eigenvalues

The refined extraction can be straightforwardly adapted to the generalized and polynomial eigenproblem (see [7]). We may also use a refined method to approximate the largest eigenvalue of these problems exploiting the modified polynomial $\widetilde{p}$ (4.2). The resulting extraction determines an approximate eigenvector by

$$u = \underset{\widetilde{u}\in\mathcal{U},\ \|\widetilde{u}\|=1}{\operatorname{argmin}} \ \|\widetilde{p}\,(\tau^{-1})u\|,$$

where τ may be any sensible target, including ∞. As usual in refined approaches, the main disadvantage of this approach is that if the sought eigenvector x is in the search space $\mathcal{U}$, the refined approach will generally fail to select it. We may start with this and extraction method and replace it by another if the process starts to converge; see also the discussion in [7].

5.4. Preconditioning. Counterintuitively, eigenvalue processes may sometimes have less trouble finding interior eigenvalues than finding exterior eigenvalues (cf., for instance, [5]). The main reason for this is that interior eigenvalues often have a clear target and therefore also a suggestive reasonable preconditioner (for instance, an inexact LU decomposition (ILU) of $p(\tau)$).

For exterior eigenvalues, one often hardly has a sensible target. For example, for standard eigenvalue problems $Ax = \lambda x$ we may take any norm of A as a guess for the largest eigenvalue, but this may be a gross overestimate, and it only predicts the magnitude, but not the complex argument, of the largest eigenvalue. For the generalized eigenvalue problems $Ax = \lambda Bx$ and $p(\lambda)\, x = 0$, a cheap guess is even more complicated. This may be another advantage of computing the smallest eigenvalues of $\widetilde{p}(\mu)\, x = 0$ instead of the largest of $p(\lambda)\, x = 0$; see the numerical experiments.

6. Numerical experiments. We will now perform numerical experiments to test (in this order)

- the relative harmonic approach of Section 2 in Experiments 6.1 and 6.2;
- the harmonic variant to compute the rightmost eigenvalue described in Section 3 in Experiment 6.3;
- the harmonic variant to compute the largest eigenvalue of Section 4 (Experiments 6.4 and 6.5), also in the presence of infinite eigenvalues (Experiment 6.6).

EXPERIMENT 6.1. Our first experiment considers three matrices with known eigenvalues:

- $A = \texttt{diag}(1{:}100)$ with target $\tau = 50.5$;
- $A = \texttt{triu}(1{:}100)$ with target $\tau = 50.5$;

- A = triu(1:1000) with target $\tau = 500.5$ and an ILU preconditioning with 0.01 fill-in.

Here, triu stands for an upper triangular matrix with random elements from the interval $[-0.5, 0.5]$ with given eigenvalues. We compare the Jacobi–Davidson (JD) method with the standard harmonic extraction with JD with the relative harmonic extraction for the same set of 100 random initial vectors. In Table 5.1 we give the percentage of cases where the methods converged towards $\lambda = 51$ and $\lambda = 50$, respectively $\lambda = 501$ and $\lambda = 500$.

TABLE 6.1: Percentage of the cases in which convergence to $\lambda = 51$ (first element) and $\lambda = 50$ (second element), resp. $\lambda = 501$ (first element) and $\lambda = 500$ (second element), occurred for a 100×100 diagonal and tridiagonal, and a 1000×1000 tridiagonal matrix and JD with the harmonic and relative harmonic approach, each with the same set of 100 random initial vectors.

Method	diag(1:100)	triu(1:100)	triu(1:1000)
Harmonic	(50, 50)%	(48, 52)%	(49, 51)%
Relative harmonic	(91, 9)%	(69, 31)%	(70, 30)%

As expected, the standard harmonic extraction finds $\lambda = 51$ and $\lambda = 50$ (resp. $\lambda = 501$ and $\lambda = 500$) in roughly half the number of cases. The relative harmonic approach detects the eigenvalue $\lambda = 51$ (resp. $\lambda = 501$) that is relatively closest to τ in the majority of the cases; the effect for the nonnormal matrices is less pronounced than for the normal matrix.

EXPERIMENT 6.2. Next, we take the following polynomial eigenproblem:

- A_2 a random diagonal matrix with elements between $(0, 1)$ (hence symmetric positive definite);
- A_1 a random skew-symmetric matrix with elements between $[-0.5, 0.5]$;
- A_0 a random diagonal matrix with elements between $(-1, 0)$ (hence symmetric negative definite).

This type of problem is typical for a gyroscopic dynamical system; all matrices are 100×100.

Our target $\tau \approx 1.53 \cdot 10^{-2} i$ is exactly between the second and third smallest eigenvalue on the positive imaginary axis. In 10 runs with different initial vectors, the harmonic approach finds 9 times the second smallest $\lambda_2 \approx 1.40 \cdot 10^{-2}$ with once no convergence. The relative harmonic approach finds 8 times the third smallest $\lambda_3 \approx 1.66 \cdot 10^{-2}$ with twice no convergence; we note that indeed λ_3 is the eigenvalue relatively closest to the target τ. However, in spite of the small sizes, the relative harmonic approach converges slowly and the final result is less accurate. This may be expected due to the fact that an exact eigenpair does not satisfy (2.8) in general.

EXPERIMENT 6.3. Let us try out the harmonic extraction for the rightmost eigenvalue (3.1). We take A = `mhd416a.mtx`, B = `mhd416b.mtx` from the Matrix Market [10]. The JD method where we take the rightmost eigenvalue in each step does not converge to any eigenvalue. The harmonic approach (3.1) with target $\tau = 2$ to find the rightmost eigenvalue ($\lambda = 1$ with multiplicity 7) quickly detects the correct eigenvalue, only the asymptotic convergence is very slow: the norm of the residual is $4.5 \cdot 10^{-2}$ after 20 steps, $1.0 \cdot 10^{-2}$ after 40 steps, but only $3.9 \cdot 10^{-3}$ after 1000 steps.

EXPERIMENT 6.4. We now demonstrate the use of the harmonic extraction (4.1) for the largest eigenvalue. We take the matrices A = `bcsstk07.mtx`, B =

bcsstm07.mtx from the Matrix Market. This 420×420 generalized eigenproblem is challenging since the largest eigenvalues $\lambda_1 \approx 1.0253 \cdot 10^8$, $\lambda_2 \approx 1.0149 \cdot 10^8$, $\lambda_5 \approx 1.0125 \cdot 10^8$, $\lambda_4 \approx 1.0120 \cdot 10^8$, $\lambda_5 \approx 1.0089 \cdot 10^8$, $\ldots$ are relatively clustered. Standard JD with the standard Ritz extraction does not converge for any of 10 random starting vectors, while JD with the harmonic extraction (4.1) for large singular vectors with an ILU-preconditioner for B (with 0.01 fill-in) converges to the largest eigenvalue in all 10 cases. Note that as discussed in Section 5.4, an important advantage of using a harmonic approach here is that we have a good target value for a preconditioner.

EXPERIMENT 6.5. We take the same example as [1, Ex. 1]: $A_2 = 0.1 \cdot I$, $A_1 = I$,

$$A_0 = \begin{bmatrix} 0.2 & -0.1 & & & \\ -0.1 & 0.2 & -0.1 & & \\ & \ddots & \ddots & \ddots & \\ & & -0.1 & 0.2 & -0.1 \\ & & & -0.1 & 0.1 \end{bmatrix}$$

but with dimension 1000×1000. We compare JD with the standard extraction to find the largest eigenvalue $\lambda \approx -10$ with JD with the harmonic extraction with target 0 on the modified problem $(A_2 + \mu A_1 + \mu^2 A_0)\, x = 0$. Both methods find the correct eigenvalue in each of 10 cases with different random initial vectors, but the latter approach is on average much faster than the first (mean number of matrix-vector multiplications: 4131 versus 1006). Note that the second approach has the additional advantage that we have a natural target to form a preconditioner, which we have not used in this example.

EXPERIMENT 6.6. Next, we illustrate the use of the relative harmonic extraction to find the largest *finite* eigenvalue. We take $A = \texttt{triu}(1{:}1000)$ and $B = I$ except for the $(1,1)$-coordinate which we set to zero. Therefore the eigenvalues of the pencil (A, B) are $\infty, 1000, 999, \ldots, 2$. Standard JD where we take the largest Ritz pair in every step does not converge, hindered by the infinite eigenvalue. The two (mathematically equivalent but practically somewhat different) harmonic approaches described in Section 4.3 with target $\tau = 10^{-4}$ converges to the largest finite eigenvalue $\lambda = 1000$. Note that $\tau^{-1} = 10^4$ is not a very accurate approximation to the largest finite eigenvalue.

7. Conclusions. We have seen that the harmonic extraction can be generalized to compute

- eigenvalues that are closest to a target in a relative sense;
- rightmost eigenvalues; and
- large eigenvalues, also in the presence of infinite eigenvalues.

The extraction processes are stand-alone methods and can be incorporated in a subspace method as Arnoldi (see, e.g., [1, 17]) or Jacobi–Davidson (see [7, 14, 15]). Since the extraction approaches consists of low-dimensional operations, the extra costs are very small; no extra matrix-vector multiplications are required.

For the generalized eigenproblem the approaches are theoretically and numerically very sound, with several connections to the standard harmonic extraction. For the polynomial eigenproblem, several proposed methods use a linearization of this polynomial. This has the effect that the method may fail to extract an exact eigenvector; in this case more modest results may be expected. A linearized method may also be combined with a non-linearized method in the sense that we may perform a non-linearized extraction if we are close to convergence; see also [7]. Another option would be to first linearize the polynomial eigenproblem into a generalized eigenproblem and subsequently use harmonic approaches for the resulting pencil.

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