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ETNA
Kent State University
etna@mcs.kent.edu

HARMONIC RAYLEIGH–RITZ EXTRACTION FOR THE MULTIPARAMETER EIGENVALUE PROBLEM*

MICHIEL E. HOCHSTENBACH† AND BOR PLESTENJAK‡

Abstract. We study harmonic and refined extraction methods for the multiparameter eigenvalue problem. These techniques are generalizations of their counterparts for the standard and generalized eigenvalue problem. The methods aim to approximate interior eigenpairs, generally more accurately than the standard extraction does. We study their properties and give Saad-type theorems. The processes can be combined with any subspace expansion approach, for instance a Jacobi–Davidson type technique, to form a subspace method for multiparameter eigenproblems of high dimension.

Key words. multiparameter eigenvalue problem, two-parameter eigenvalue problem, harmonic extraction, refined extraction, Rayleigh–Ritz, subspace method, Saad's theorem, Jacobi–Davidson

AMS subject classifications. 65F15, 65F50, 15A18, 15A69

1. Introduction.

We study harmonic and refined Rayleigh–Ritz techniques for the multiparameter eigenvalue problem (MEP). For ease of presentation we will focus on the two-parameter eigenvalue problem

$$\begin{aligned} A_1x &= \lambda B_1x + \mu C_1x,\\ A_2y &= \lambda B_2y + \mu C_2y, \end{aligned} \tag{1.1}$$

for given $n_1 \times n_1$ (real or complex) matrices A_1, B_1, C_1, and $n_2 \times n_2$ matrices A_2, B_2, C_2; we are interested in eigenpairs $((\lambda, \mu),\ x \otimes y)$ where x and y have unit norm. The approaches for general multiparameter eigenproblems will be straightforward generalizations of the two-parameter case.

Multiparameter eigenvalue problems of this kind arise in a variety of applications [1], particularly in mathematical physics when the method of separation of variables is used to solve boundary value problems [27]; see [10] for several other applications.

Two-parameter problems can be expressed as two coupled generalized eigenvalue problems as follows. On the tensor product space $\mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2}$ of dimension n_1n_2, one defines the matrix determinants

$$\begin{aligned} \Delta_0 &= B_1 \otimes C_2 - C_1 \otimes B_2,\\ \Delta_1 &= A_1 \otimes C_2 - C_1 \otimes A_2,\\ \Delta_2 &= B_1 \otimes A_2 - A_1 \otimes B_2. \end{aligned} \tag{1.2}$$

The MEP is called *right definite* if all the $A_i, B_i, C_i,\ i = 1, 2$, are Hermitian and Δ_0 is (positive or negative) definite; in this case the eigenvalues are real and the eigenvectors can be chosen to be real. The MEP is called *nonsingular* if Δ_0 is nonsingular (without further conditions on the A_i, B_i, C_i). A nonsingular two-parameter eigenvalue problem is equivalent

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†Department of Mathematics and Computing Science, Eindhoven University of Technology, PO Box 513, 5600 MB, The Netherlands (www.win.tue.nl/∼hochsten/). The research of this author was supported in part by NSF grant DMS-0405387.

‡Department of Mathematics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia (www-lp.fmf.uni-lj.si/plestenjak/bor.htm).

to the coupled generalized eigenvalue problems

$$\begin{aligned} \Delta_1 z &= \lambda \Delta_0 z, \\ \Delta_2 z &= \mu \Delta_0 z, \end{aligned} \tag{1.3}$$

where $z = x \otimes y$, and $\Delta_0^{-1}\Delta_1$ and $\Delta_0^{-1}\Delta_2$ commute. Because of the product dimension $n_1 n_2$, the multiparameter eigenvalue problem is a computationally quite challenging problem.

There exist several numerical methods for the MEP. Blum and colleagues [2, 3, 4], Bohte [5], and Browne and Sleeman [6] proposed methods for computing one eigenvalue, hopefully the closest one to a given approximation. There are also methods which determine all eigenvalues. The first class is formed by *direct methods* for right definite MEPs [24, 14, 7] and for non right definite MEPs [10]; these methods are suitable for small (dense) matrices only since their complexity is $\mathcal{O}((n_1 n_2)^3)$. The second class consists of continuation methods [23, 19, 20] that are asymptotically somewhat cheaper than direct methods, but are so far often not very competitive for small problems in practice; for larger problems their computational cost is still enormous.

Fortunately, in applications often only a few relevant eigenpairs are of interest, for instance those corresponding to the largest eigenvalues, or the eigenvalues closest to a given target. Recently some subspace methods for the MEP have been proposed [11, 10] that are suitable for finding some selected eigenpairs. These methods combine a subspace approach with one of the mentioned dense methods as solver for the projected MEP. The approaches are also suitable for multiparameter problems where the matrices are large and sparse, although convergence to the wanted eigenpairs may sometimes remain an issue of concern. In particular, in [11] it was observed that finding interior eigenvalues was one of the challenges for the Jacobi–Davidson type method. It was left as an open question how to generalize the harmonic Rayleigh–Ritz approach for the MEP. This paper addresses this issue, and also introduces a refined Ritz method.

The rest of the paper has been organized as follows. In Section 2 we review the harmonic Rayleigh–Ritz method for the generalized eigenproblem, after which this method is generalized for the MEP in Section 3. In Section 4 we present two Saad-type theorems for the standard and harmonic extraction. Section 5 proposes a refined Rayleigh–Ritz method for the MEP. We conclude with experiments and a conclusion in Sections 6 and 7.

2. Harmonic Rayleigh–Ritz for the generalized eigenvalue problem. We first briefly review the harmonic Rayleigh–Ritz for the generalized eigenvalue problem

$$Ax = \lambda Bx.$$

Suppose we would like to compute an approximation (θ, u) to the eigenpair (λ, x), where the approximate eigenvector u should be in a given search space $\mathcal{U}_k$ of low dimension k, and θ should be in the neighborhood of the target $\tau \in \mathbb{C}$.

Since $u \in \mathcal{U}_k$, we can write $u = U_k c$, where the columns of U_k form an orthonormal basis for $\mathcal{U}_k$, and c is a vector in $\mathbb{C}^k$ of unit norm. The standard Ritz–Galerkin condition on the residual r is (cf. [18])

$$r := Au - \theta Bu \perp \mathcal{U}_k,$$

which implies that (θ, c) should be a primitive Ritz pair (terminology from Stewart [26]), an eigenpair of the projected generalized eigenproblem

$$U_k^* A U_k c = \theta\, U_k^* B U_k c.$$

It follows that if $u^*Bu \neq 0$, then $\theta = \frac{u^*Au}{u^*Bu}$; the case $u^*Bu = 0$ is an exceptional case where the Ritz value is infinite (if $u^*Au \neq 0$) or undefined (if $u^*Au = 0$). If B is Hermitian positive definite, then we can define the B^{-1}-norm of the residual by $\|z\|_{B^{-1}}^2 = z^*B^{-1}z$, and one can show that this θ minimizes $\|r\|_{B^{-1}}$.

However, the problem with this standard Rayleigh–Ritz approach is that even if there is a Ritz value $\theta \approx \tau$, we do not have the guarantee that the two-norm $\|r\|$ is small, which reflects the fact that the approximate eigenvector may be poor. As a remedy, the harmonic Rayleigh–Ritz was proposed by Morgan [16], Paige, Parlett, and Van der Vorst [17] for the standard eigenproblem, and by Stewart [26] for the generalized eigenproblem; see also Fokkema, Sleijpen, and Van der Vorst [9]. Assuming $A - \tau B$ is nonsingular, the idea is to consider a spectral transformation

$$(A - \tau B)^{-1} Bx = (\lambda - \tau)^{-1} x. \tag{2.1}$$

Thus, the interior eigenvalues $\lambda \approx \tau$ are exterior eigenvalues of $(A - \tau B)^{-1}B$ for which a Galerkin condition usually works well in practice. To avoid working with $(A - \tau B)^{-1}$, the inverse of a large sparse matrix, we impose a Petrov–Galerkin condition

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

or, equivalently,

$$Au - \theta Bu = (A - \tau B)\,u - (\theta - \tau)\,Bu \perp (A - \tau B)\,\mathcal{U}_k, \tag{2.2}$$

leading to the projected eigenproblem

$$U_k^*(A - \tau B)^*(A - \tau B)\,U_k c = (\theta - \tau)\,U_k^*(A - \tau B)^* BU_k c. \tag{2.3}$$

Here we are interested in the primitive harmonic Ritz pair(s) (θ, c) with θ closest to τ. This approach has two motivations:

- if an exact eigenvector is in the search space, $x = U_k c$, then the eigenpair (λ, x) satisfies (2.3) (this implies that exact eigenvectors in the search space will be detected unless we are in the special circumstance of the presence of multiple harmonic Ritz values);
- a harmonic Ritz pair (θ, u) satisfies

$$\|Au - \tau Bu\| \leq |\theta - \tau| \cdot \|Bu\| \leq |\theta - \tau| \cdot \|BU_k\|$$

(see, e.g., [26]) which motivates the choice of the harmonic Ritz value closest to τ.

The harmonic Rayleigh–Ritz approach was generalized for the polynomial eigenproblem in [13].

3. Harmonic Rayleigh–Ritz for the multiparameter eigenvalue problem. For the MEP (1.1) it is natural to make use of two search spaces, $\mathcal{U}_k$ and $\mathcal{V}_k$, for the vectors x and y, respectively. Let the columns of U_k and V_k form orthonormal bases for $\mathcal{U}_k$ and $\mathcal{V}_k$. We look for an approximate eigenpair $((\theta, \eta),\ u \otimes v) \approx ((\lambda, \mu), x \otimes y)$, where $u \otimes v$ is of the form $U_k c \otimes V_k d$, where both $c, d \in \mathbb{C}^k$ are of unit norm. The standard extraction,

$$\begin{aligned} (A_1 - \theta B_1 - \eta C_1)\,U_k c &\perp \mathcal{U}_k, \\ (A_2 - \theta B_2 - \eta C_2)\,V_k d &\perp \mathcal{V}_k \end{aligned} \tag{3.1}$$

was introduced in [11]. As is also the case for the standard eigenvalue problem, the standard extraction for the MEP works well for exterior eigenvalues, but is generally less favorable for interior ones [11].

ETNA
Kent State University
etna@mcs.kent.edu

Now suppose we are interested in a harmonic approach to better approximate eigenpairs near the target (σ, τ). One obstacle is that MEPs do not seem to allow for a straightforward generalization of the spectral transformation (2.1). Therefore we generalize (2.2) and impose the two Galerkin conditions

$$\begin{aligned} (A_1 - \theta B_1 - \eta C_1)\, u &\perp (A_1 - \sigma B_1 - \tau C_1)\, \mathcal{U}_k, \\ (A_2 - \theta B_2 - \eta C_2)\, v &\perp (A_2 - \sigma B_2 - \tau C_2)\, \mathcal{V}_k, \end{aligned} \tag{3.2}$$

or, equivalently,

$$\begin{aligned} (A_1 - \sigma B_1 - \tau C_1)\, U_k c - (\theta - \sigma)\, B_1 U_k c - (\eta - \tau)\, C_1 U_k c &\perp (A_1 - \sigma B_1 - \tau C_1)\, \mathcal{U}_k, \\ (A_2 - \sigma B_2 - \tau C_2)\, V_k d - (\theta - \sigma)\, B_2 V_k d - (\eta - \tau)\, C_2 V_k d &\perp (A_2 - \sigma B_2 - \tau C_2)\, \mathcal{V}_k. \end{aligned}$$

We call this the harmonic Rayleigh–Ritz extraction for the MEP. Introduce the following reduced QR-decompositions

$$(A_1 - \sigma B_1 - \tau C_1)\, U_k = Q_1 R_1, \qquad (A_2 - \sigma B_2 - \tau C_2)\, V_k = Q_2 R_2, \tag{3.3}$$

which we can compute incrementally, i.e., one column per step, during the subspace method. This is done for computational efficiency, as well as stability: cross products of the form $(A_i - \sigma B_i - \tau C_i)^*(A_i - \sigma B_i - \tau C_i)$ with potentially a high condition number are avoided. Then, computationally, the extraction amounts to the projected two-parameter eigenproblem

$$\begin{aligned} R_1\, c &= (\theta - \sigma)\, Q_1^* B_1 U_k c + (\eta - \tau)\, Q_1^* C_1 U_k c, \\ R_2\, d &= (\theta - \sigma)\, Q_2^* B_2 V_k d + (\eta - \tau)\, Q_2^* C_2 V_k d. \end{aligned}$$

We now compute the smallest eigenpair(s) $((\xi_1, \xi_2),\ c \otimes d)$ (in absolute value sense, that is, with minimal $|\xi_1|^2 + |\xi_2|^2$) of the low-dimensional MEP

$$\begin{aligned} R_1\, c &= \xi_1\, Q_1^* B_1 U_k c + \xi_2\, Q_1^* C_1 U_k c, \\ R_2\, d &= \xi_1\, Q_2^* B_2 V_k d + \xi_2\, Q_2^* C_2 V_k d, \end{aligned} \tag{3.4}$$

which can be solved by existing low-dimensional techniques as mentioned in the introduction.

As in the case for the generalized eigenproblem, there are two justifications for the harmonic approach for the MEP:

- we have the following upper bounds for the residual norms:

  $$\begin{aligned} \|(A_1 - \sigma B_1 - \tau C_1)u\| &\le |\xi_1|\, \|B_1 u\| + |\xi_2|\, \|C_1 u\| \le |\xi_1|\, \|B_1 U_k\| + |\xi_2| \|C_1 U_k\|, \\ \|(A_2 - \sigma B_2 - \tau C_2)v\| &\le |\xi_1|\, \|B_2 v\| + |\xi_2|\, \|C_2 v\| \le |\xi_1|\, \|B_2 V_k\| + |\xi_2|\, \|C_2 V_k\|, \end{aligned}$$

  so to obtain small residual norms it is clear that it is sensible to select the smallest (ξ_1, ξ_2);
- if the search spaces contain an eigenvector, $x = U_k c$, $y = V_k d$, then the pair $((\lambda, \mu), x \otimes y)$ satisfies (3.2); this means that this pair is a harmonic Ritz pair unless the harmonic Ritz value (θ, η) is not simple. We will prove a more precise statement in the next section.

In conclusion, the harmonic approach for the MEP tries to combine two desirable properties: it will generally find an exact eigenpair present in the search spaces, while it will also try to detect approximate eigenpairs with small residual norm.

4. Saad-type theorems. In this section, we derive Saad-type theorems for both the standard and harmonic extraction for the MEP. This type of theorem expresses the quality of the approximate vectors in terms of the quality of the search spaces. The original theorem by Saad [21, Thm. 4.6] was for the standard extraction for the standard Hermitian eigenvalue problem. A generalization for non-Hermitian matrices and eigenspaces was given by Stewart [25], while an extension for the harmonic extraction for the standard eigenvalue problem was presented by Chen and Jia [8].

4.1. A Saad-type theorem for the standard extraction. Let $w := u \otimes v$ be a Ritz vector corresponding to Ritz value (θ, η), and $[w \;\; W \;\; W_\perp]$ be an orthonormal basis for $\mathbb{C}^{n_1 n_2}$ such that

$$\operatorname{span}([w \;\; W]) = \mathcal{U}_k \otimes \mathcal{V}_k.$$

Define, for $i = 0, 1, 2$,

$$E_i = [w \;\; W]^* \Delta_i [w \;\; W]. \tag{4.1}$$

We assume that E_0 is invertible, which is guaranteed if Δ_0 is definite as in the case of a right definite MEP. From (3.1) we have that the Ritz pairs are of the form $((\theta, \eta), U_k c \otimes V_k d)$ where $((\theta, \eta), c \otimes d)$ are the eigenvalues of

$$\begin{aligned} U_k^* A_1 U_k c &= \theta\, U_k^* B_1 U_k c + \eta\, U_k^* C_1 U_k c, \\ V_k^* A_2 V_k d &= \theta\, V_k^* B_2 V_k d + \eta\, V_k^* C_2 V_k d. \end{aligned}$$

The three matrix determinants of this projected MEP (cf. (1.2)) are of the form $Q^* E_i Q$, where Q is the orthonormal basis transformation matrix that maps $U_k \otimes V_k$ coordinates to $[w \;\; W]$ coordinates: $Q = [w \;\; W]^* (U_k \otimes V_k)$. For instance, we have

$$\begin{aligned} U_k^* B_1 U_k \otimes V_k^* C_2 V_k - U_k^* C_1 U_k \otimes V_k^* B_2 V_k &= (U_k \otimes V_k)^* \Delta_0 (U_k \otimes V_k) \\ &= Q^* [w \;\; W]^* \Delta_0 [w \;\; W] Q = Q^* E_0 Q. \end{aligned}$$

Therefore, the components θ_j and η_j of the Ritz values (θ_j, η_j) are eigenvalues of

$$E_0^{-1} E_1 \quad \text{and} \quad E_0^{-1} E_2,$$

respectively (cf. (1.3)). In particular we know that

$$(E_1 - \theta E_0)\, e_1 = 0$$

so $E_0^{-1} E_1$ is of the form

$$E_0^{-1} E_1 = \begin{bmatrix} \theta & f_1^* \\ 0 & G_1 \end{bmatrix}, \tag{4.2}$$

where the precise expression for G_1 is less important than the fact that its eigenvalues are the $k^2 - 1$ θ_j-values belonging to the pairs (θ_j, η_j) distinct from (θ, η). We hereby note that some of the first coordinates θ_j may still be equal to θ, even if (θ, η) is not a multiple Ritz value. Similarly, $E_0^{-1} E_2$ is of the form

$$E_0^{-1} E_2 = \begin{bmatrix} \eta & f_2^* \\ 0 & G_2 \end{bmatrix}, \tag{4.3}$$

where the eigenvalues of G_2 are the k^2-1 η_j-values belonging to the pairs (θ_j, η_j) distinct from (θ, η). Using these quantities, we can now prove the following theorem, which extends [21, Thm. 4.6], [25, Thm. 2], and [8, Thm. 3].

THEOREM 4.1. *Let $((\theta,\eta),\ u\otimes v)$ be a Ritz pair and $((\lambda,\mu),\ x\otimes y)$ an eigenpair. Let $E_i = [w\ \ W]^*\Delta_i[w\ \ W]$ for $i=0,1,2$ and assume E_0 is invertible. Then*

$$\sin(u\otimes v,\ x\otimes y) \le \sqrt{1+\frac{\gamma^2}{\delta^2}}\cdot \sin(\mathcal{U}_k\otimes\mathcal{V}_k,\ x\otimes y),$$

where

$$\gamma = \|E_0^{-1}\|\cdot\Big(\|P_{\mathcal{U}_k\otimes\mathcal{V}_k}(\Delta_1-\lambda\Delta_0)(I-P_{\mathcal{U}_k\otimes\mathcal{V}_k})\|^2 + \|P_{\mathcal{U}_k\otimes\mathcal{V}_k}(\Delta_2-\mu\Delta_0)(I-P_{\mathcal{U}_k\otimes\mathcal{V}_k})\|^2\Big)^{1/2},$$

$$\delta = \sigma_{\min}\left(\begin{bmatrix} G_1-\lambda I\\ G_2-\mu I\end{bmatrix}\right),$$

and $P_{\mathcal{U}_k\otimes\mathcal{V}_k}$ is the orthogonal projection onto $\mathcal{U}_k\otimes\mathcal{V}_k$.

Proof. From $\Delta_1 z = \lambda\Delta_0 z$, where as before $z = x\otimes y$, we get with a change of variables

$$[w\ \ W\ \ W_\perp]^*(\Delta_1-\lambda\Delta_0)[w\ \ W\ \ W_\perp][a_1\ \ a_2\ \ a_3]^T = 0,$$

where

$$[a_1\ \ a_2\ \ a_3]^T = [w\ \ W\ \ W_\perp]^* z.$$

Writing out the first and second (block) equation gives

$$(E_1-\lambda E_0)\begin{bmatrix} a_1\\ a_2\end{bmatrix} = -[w\ \ W]^*(\Delta_1-\lambda\Delta_0)W_\perp a_3.$$

Left-multiplying by E_0^{-1} and using (4.2) yield

$$\begin{bmatrix} \theta-\lambda & f_1^*\\ 0 & G_1-\lambda I\end{bmatrix}\begin{bmatrix} a_1\\ a_2\end{bmatrix} = -E_0^{-1}[w\ \ W]^*(\Delta_1-\lambda\Delta_0)W_\perp\, a_3.$$

Hence,

$$\|(G_1-\lambda I)\,a_2\| \le \|E_0^{-1}[w\ \ W]^*(\Delta_1-\lambda\Delta_0)W_\perp\, a_3\|. \tag{4.4}$$

Similarly, if we start from $\Delta_2 z = \mu\Delta_0 z$ and use (4.3), we get the bound

$$\|(G_2-\mu I)\,a_2\| \le \|E_0^{-1}[w\ \ W]^*(\Delta_2-\mu\Delta_0)W_\perp\, a_3\|. \tag{4.5}$$

From (4.4) and (4.5) it follows that

$$\begin{aligned}
\sigma_{\min}\left(\begin{bmatrix} G_1-\lambda I\\ G_2-\mu I\end{bmatrix}\right)\|a_2\| &\le \left\|\begin{bmatrix} (G_1-\lambda I)\,a_2\\ (G_2-\mu I)\,a_2\end{bmatrix}\right\|\\
&\le \left\|\begin{bmatrix} E_0^{-1}[w\ \ W]^*(\Delta_1-\lambda\Delta_0)W_\perp\, a_3\\ E_0^{-1}[w\ \ W]^*(\Delta_2-\mu\Delta_0)W_\perp\, a_3\end{bmatrix}\right\|\\
&\le \|E_0^{-1}\|\,\left\|\begin{bmatrix} [w\ \ W]^*(\Delta_1-\lambda\Delta_0)W_\perp\\ [w\ \ W]^*(\Delta_2-\mu\Delta_0)W_\perp\end{bmatrix}\right\|\,\|a_3\|.
\end{aligned}$$

ETNA
Kent State University
etna@mcs.kent.edu

This gives us the bound $\|a_2\| \leq (\gamma/\delta)\,\|a_3\|$.

Since $\|a\| = 1$, we have that

$$\begin{aligned} |a_1|^2 &= \cos^2(u \otimes v,\, x \otimes y), \\ |a_1|^2 + \|a_2\|^2 &= \cos^2(\mathcal{U}_k \otimes \mathcal{V}_k,\, x \otimes y), \\ \|a_2\|^2 + \|a_3\|^2 &= 1 - \cos^2(u \otimes v,\, x \otimes y), \\ \|a_3\|^2 &= 1 - \cos^2(\mathcal{U}_k \otimes \mathcal{V}_k,\, x \otimes y). \end{aligned}$$

The result now follows from substituting the bound for $\|a_2\|$ in terms of $\|a_3\|$ in the expression $\|a_2\|^2 + \|a_3\|^2$. $\square$

The significance of the theorem is the following. If $\sin(\mathcal{U}_k \otimes \mathcal{V}_k,\, x \otimes y) \to 0$, we know that $\sin(u \otimes v,\, x \otimes y) \to 0$, so there is a Ritz vector $u \otimes v$ converging to the eigenvector $x \otimes y$—unless δ is zero, which means that (λ, μ) coincides with one of the Ritz values distinct from (θ, η).

4.2. A Saad-type theorem for the harmonic extraction. We have a similar theorem for the harmonic extraction, *mutatis mutandis*, which means that the harmonic extraction is also asymptotically accurate. Define the quantities

$$\begin{aligned} \widetilde{A}_i &= (A_i - \sigma B_i - \tau C_i)^* A_i, & \widetilde{\Delta}_0 &= \widetilde{B}_1 \otimes \widetilde{C}_2 - \widetilde{C}_1 \otimes \widetilde{B}_2, \\ \widetilde{B}_i &= (A_i - \sigma B_i - \tau C_i)^* B_i, & \widetilde{\Delta}_1 &= \widetilde{A}_1 \otimes \widetilde{C}_2 - \widetilde{C}_1 \otimes \widetilde{A}_2, \\ \widetilde{C}_i &= (A_i - \sigma B_i - \tau C_i)^* C_i, & \widetilde{\Delta}_2 &= \widetilde{B}_1 \otimes \widetilde{A}_2 - \widetilde{A}_1 \otimes \widetilde{B}_2. \end{aligned}$$

Let $\widetilde{w} := \widetilde{u} \otimes \widetilde{v}$ be a harmonic Ritz vector corresponding to the harmonic Ritz value $(\widetilde{\theta}, \widetilde{\eta})$, and let $[\widetilde{w}\ \ \widetilde{W}\ \ W_\perp]$ be an orthonormal basis for $\mathbb{C}^{n_1 n_2}$ such that $\mathrm{span}([\widetilde{w}\ \ \widetilde{W}]) = \mathcal{U}_k \otimes \mathcal{V}_k$.

Similar to (4.1), define, $\widetilde{E}_i = [\widetilde{w}\ \ \widetilde{W}]^* \widetilde{\Delta}_i [\widetilde{w}\ \ \widetilde{W}]$ for $i = 0, 1, 2$. Then the components $\widetilde{\theta}_j$ and $\widetilde{\eta}_j$ of the harmonic Ritz values $(\widetilde{\theta}_j, \widetilde{\eta}_j)$ are eigenvalues of $\widetilde{E}_0^{-1}\widetilde{E}_1$ and $\widetilde{E}_0^{-1}\widetilde{E}_2$, respectively. Since $(\widetilde{E}_1 - \widetilde{\theta}\widetilde{E}_0)\, e_1 = 0$ we know that $\widetilde{E}_0^{-1}\widetilde{E}_1$ is of the form

$$\widetilde{E}_0^{-1}\widetilde{E}_1 = \begin{bmatrix} \widetilde{\theta} & \widetilde{f}_1^* \\ 0 & \widetilde{G}_1 \end{bmatrix},$$

where the eigenvalues of $\widetilde{G}_1$ are the $k^2 - 1$ $\widetilde{\theta}_j$-values belonging to the pairs $(\widetilde{\theta}_j, \widetilde{\eta}_j)$ distinct from $(\widetilde{\theta}, \widetilde{\eta})$. Similarly, $\widetilde{E}_0^{-1}\widetilde{E}_2$ is of the form

$$\widetilde{E}_0^{-1}\widetilde{E}_2 = \begin{bmatrix} \widetilde{\eta} & \widetilde{f}_2^* \\ 0 & \widetilde{G}_2 \end{bmatrix},$$

where the eigenvalues of $\widetilde{G}_2$ are the $k^2 - 1$ $\widetilde{\eta}_j$-values belonging to the pairs $(\widetilde{\theta}_j, \widetilde{\eta}_j)$ distinct from $(\widetilde{\theta}, \widetilde{\eta})$. Analogous to Theorem 4.1 we can prove the following result.

THEOREM 4.2. *Let $((\widetilde{\theta}, \widetilde{\eta}),\ \widetilde{u} \otimes \widetilde{v})$ be a harmonic Ritz pair and $((\lambda, \mu),\ x \otimes y)$ be an eigenpair. Let $\widetilde{E}_i = [\widetilde{w}\ \ \widetilde{W}]^* \Delta_i [\widetilde{w}\ \ \widetilde{W}]$ for $i = 0, 1, 2$ and assume $\widetilde{E}_0$ is invertible. Then*

$$\sin(\widetilde{u} \otimes \widetilde{v},\, x \otimes y) \leq \sqrt{1 + \frac{\widetilde{\gamma}^2}{\widetilde{\delta}^2}} \cdot \sin(\mathcal{U}_k \otimes \mathcal{V}_k,\, x \otimes y),$$

ETNA
Kent State University
etna@mcs.kent.edu

where

$$\widetilde{\gamma} = \|\widetilde{E}_0^{-1}\| \cdot \Big(\|P_{\mathcal{U}_k\otimes\mathcal{V}_k}(\widetilde{\Delta}_1 - \lambda\widetilde{\Delta}_0)(I - P_{\mathcal{U}_k\otimes\mathcal{V}_k})\|^2 + \|P_{\mathcal{U}_k\otimes\mathcal{V}_k}(\widetilde{\Delta}_2 - \mu\widetilde{\Delta}_0)(I - P_{\mathcal{U}_k\otimes\mathcal{V}_k})\|^2 \Big)^{1/2},$$

$$\widetilde{\delta} = \sigma_{\min}\left(\begin{bmatrix} \widetilde{G}_1 - \lambda I \\ \widetilde{G}_2 - \mu I \end{bmatrix} \right).$$

This means that if $\sin(\mathcal{U}_k \otimes \mathcal{V}_k,\ x \otimes y) \to 0$, then there is a harmonic Ritz vector $\widetilde{u} \otimes \widetilde{v}$ converging to the eigenvector $x \otimes y$—unless (λ, μ) coincides with one of the harmonic Ritz values distinct from $(\widetilde{\theta}, \widetilde{\eta})$.

Comparing Theorems (4.1) and (4.2), we see that both the standard and harmonic extraction are asymptotically accurate: up to the occurrence of multiple (harmonic) Ritz values, they will recognize an eigenvector present in the search space.

5. Refined extraction for the multiparameter problem. The refined extraction is an alternative approach that minimizes the residual norm over a given search space. It was popularized for the standard eigenvalue problem by Jia [15]. We now generalize this approach for the MEP.

Given σ and τ, for instance a tensor Rayleigh quotient [19] of the form

$$\begin{aligned} \sigma &= \frac{(u\otimes v)^*\Delta_1(u\otimes v)}{(u\otimes v)^*\Delta_0(u\otimes v)} = \frac{(u^*A_1u)(v^*C_2v) - (u^*C_1u)(v^*A_2v)}{(u^*B_1u)(v^*C_2v) - (u^*C_1u)(v^*B_2v)}, \\ \tau &= \frac{(u\otimes v)^*\Delta_2(u\otimes v)}{(u\otimes v)^*\Delta_0(u\otimes v)} = \frac{(u^*B_1u)(v^*A_2v) - (u^*A_1u)(v^*B_2v)}{(u^*B_1u)(v^*C_2v) - (u^*C_1u)(v^*B_2v)}, \end{aligned} \tag{5.1}$$

or a target, the refined extraction determines an approximate eigenvector $\widehat{u}\otimes\widehat{v}$ by minimizing the residual norms over $\mathcal{U}_k$ and $\mathcal{V}_k$, respectively:

$$\begin{aligned} \widehat{u} &= \underset{u\in\mathcal{U}_k,\ \|u\|=1}{\operatorname{argmin}} \ \|(A_1 - \sigma B_1 - \tau C_1)\,u\|, \\ \widehat{v} &= \underset{v\in\mathcal{V}_k,\ \|v\|=1}{\operatorname{argmin}} \ \|(A_2 - \sigma B_2 - \tau C_2)\,v\|. \end{aligned} \tag{5.2}$$

In practice, it is often sensible to take the target in the beginning of the process, and switch to the Rayleigh quotient when the residual norm is under a certain threshold, because this indicates that the Rayleigh quotient is of sufficient quality.

If we always use the same target, then (5.2) is computationally best determined by two incremental QR-decompositions (3.3), followed by singular value decompositions of R_1 and R_2. If we vary σ and τ during the process, then we may incrementally compute QR-like decompositions

$$\begin{array}{lllllllll} A_1U_k &=& \widetilde{Q}_1R_{1A}, & B_1U_k &=& \widetilde{Q}_1R_{1B}, & C_1U_k &=& \widetilde{Q}_1R_{1C}, \\ A_2V_k &=& \widetilde{Q}_2R_{2A}, & B_2V_k &=& \widetilde{Q}_2R_{2B}, & C_2V_k &=& \widetilde{Q}_2R_{2C}, \end{array}$$

where $\widetilde{Q}_1$ and $\widetilde{Q}_2$ have $3k$ orthonormal columns and R_{1A}, R_{1B}, R_{1C}, R_{2A}, R_{2B}, and R_{2C} are $3k \times k$ matrices. Such decompositions can be computed efficiently with a straightforward generalization of the approach presented in [22] for the case of two matrices. For each different value of σ and τ we then evaluate (5.2) by QR-decompositions of the $3k \times k$ matrices $R_{1A} - \sigma R_{1B} - \tau R_{1C}$ and $R_{2A} - \sigma R_{2B} - \tau R_{2C}$, followed by singular value decompositions of $k \times k$ upper triangular matrices.

ETNA
Kent State University
etna@mcs.kent.edu

The following theorem is a generalization of [26, Thm. 4.10].

THEOREM 5.1. *For the residuals of the refined Ritz vector (5.2) we have*

$$\|(A_1 - \sigma B_1 - \tau C_1)\widehat{u}\| \le \frac{|\lambda - \sigma|\|B_1\| + |\mu - \tau|\|C_1\| + \|(A_1 - \sigma B_1 - \tau C_1)\| \sin(\mathcal{U}_k, x)}{\sqrt{1 - \sin^2(\mathcal{U}_k, x)}},$$

$$\|(A_2 - \sigma B_2 - \tau C_2)\widehat{v}\| \le \frac{|\lambda - \sigma|\|B_2\| + |\mu - \tau|\|C_2\| + \|(A_2 - \sigma B_2 - \tau C_2)\| \sin(\mathcal{V}_k, y)}{\sqrt{1 - \sin^2(\mathcal{V}_k, y)}}.$$

Proof. Decompose $x = \gamma_U x_U + \sigma_U e_U$, where $x_U := UU^*x \,/\, \|UU^*x\|$ is the orthogonal projection of x onto $\mathcal{U}$, $\|x_U\| = \|e_U\| = 1$, $\gamma_U = \cos(\mathcal{U}_k, x)$, and $\sigma_U = \sin(\mathcal{U}_k, x)$. Since $x_U = (x - \sigma_U e_U)/\gamma_U$, we have by the definition of a refined Ritz vector (5.2)

$$\begin{aligned} \|(A_1 - \sigma B_1 - \tau C_1)\,\widehat{u}\| &\le \|(A_1 - \sigma B_1 - \tau C_1)\,x_U\| \\ &\le \|(\lambda - \sigma)\,B_1 x + (\mu - \tau)\,C_1 x + \sigma_U\,(A_1 - \sigma B_1 - \tau C_1)\,e_U\|/\gamma_U, \end{aligned}$$

from which the first result follows. The derivation of the second result is similar. □

Similar to the refined extraction for the standard eigenvalue problem we see that, in contrast to the situation for the standard and harmonic extraction methods (Theorems 4.1 and 4.2), the conditions $\sin(\mathcal{U}_k, x) \to 0$ and $\sin(\mathcal{V}_k, y) \to 0$ are no longer sufficient for convergence of the refined vectors to eigenvectors; we also need $\sigma \to \lambda$ and $\tau \to \mu$.

Recall from Theorem 4.1 that if an eigenvalue is simple, then $\sin(\mathcal{U}_k, x) \to 0$ and $\sin(\mathcal{V}_k, y) \to 0$ imply that there is a Ritz vector converging to the eigenvector corresponding to that eigenvalue. From this follows in turn that the Ritz value converges to the eigenvalue; see, e.g., [11]. Therefore, if we are prepared to accept additional computational costs by varying σ and τ and asymptotically take the Ritz value as shifts, the refined Ritz vector will converge to the eigenvector if the eigenvalue is simple and $\sin(\mathcal{U}_k, x) \to 0$ and $\sin(\mathcal{V}_k, y) \to 0$.

6. Numerical experiments. The numerical results in this section were obtained with Matlab 7.0.

EXAMPLE 6.1. In the first example we consider a random right definite two-parameter eigenvalue problems with known eigenpairs, which enables us to check the obtained results. We take

$$A_i = S_i F_i S_i^*, \quad B_i = S_i G_i S_i^*, \quad C_i = S_i H_i S_i^*,$$

where F_i, G_i, and H_i are diagonal matrices and S_i are banded matrices generated in Matlab by `2*speye(1000)+triu(tril(sprandn(1000,1000,d),b),-b)`, where d is the density and b is the bandwidth for $i = 1, 2$. We select the diagonal elements of F_1, F_2, G_2, and H_1 as normally distributed random numbers with mean zero, variance one and standard deviation one, and the diagonal elements of G_1 and H_2 as normally distributed random numbers with mean 5, variance one and standard deviation one. In this way, the problem is right definite and the eigenvalues can be computed exactly from diagonal elements of F_i, G_i, and H_i, see [11] for details.

We are interested in approximating the innermost eigenpair $((\lambda, \mu), x \otimes y)$, i.e., the pair for which the eigenvalue (λ, μ) is closest to the arithmetic mean of the eigenvalues. For the search subspace $\mathcal{U}$ we take the span of $\widetilde{x}$, which is a perturbation of the eigenvector component x, and nine additional random vectors. The search space $\mathcal{V}$ is formed similarly.

ETNA
Kent State University
etna@mcs.kent.edu

We test with different perturbations which affect the quality of the 10-dimensional search spaces $\mathcal{U}$ and $\mathcal{V}$. We compare the approximations for the innermost eigenpair obtained from the standard and the harmonic extraction. The results are in Table 6.1. Let (θ,η) be a standard or harmonic Ritz value that approximates (λ,μ) and let $u\otimes v$ be the corresponding standard or harmonic Ritz vector. The rows in Table 6.1 are:

- *subspace*: $\angle(x\otimes y,\,\mathcal{U}\otimes\mathcal{V})$, the angle between the exact eigenvector $x\otimes y$ and the search subspace $\mathcal{U}\otimes\mathcal{V}$; this quantity indicates the best result any extraction method can obtain.
- *vector*: $\angle(u\otimes v,\ x\otimes y)$, the angle between the exact eigenvector and the (harmonic) Ritz vector.
- *value*: $(|\lambda-\theta|^2+|\mu-\eta|^2)^{1/2}$, the difference between the (harmonic) Ritz value (θ,η) and the exact eigenvalue (λ,μ).
- *residual*: the norm of the residual of the (harmonic) Ritz pair

$$\left(\|(A_1-\theta B_1-\eta C_1)\,u\|^2+\|(A_2-\theta B_2-\eta C_2)\,v\|^2\right)^{1/2}.$$

- *RQ value*: the difference between the Rayleigh quotient (5.1) of the (harmonic) Ritz vector and the exact eigenvalue (λ,μ). Note that for the standard extraction this is the same as the *value* column and therefore omitted.
- *RQ residual*: the norm of the residual

$$\left(\|(A_1-\theta B_1-\eta C_1)\,u\|^2+\|(A_2-\theta B_2-\eta C_2)\,v\|^2\right)^{1/2},$$

  where we take the Rayleigh quotient of the (harmonic) Ritz vector instead of the (harmonic) Ritz value. Note that for the standard extraction this is the same as the *residual* column.
- *refined vector*: $\angle(\widehat{u}\otimes\widehat{v},\ x\otimes y)$, the angle between the exact eigenvector and the refined vector $\widehat{u}\otimes\widehat{v}$, which minimizes (5.2) with the Ritz value, respectively with the Rayleigh quotient of the harmonic Ritz vector as shift.
- *refined residual*: the norm of the residual

$$\left(\|(A_1-\theta B_1-\eta C_1)\,\widehat{u}\|^2+\|(A_2-\theta B_2-\eta C_2)\,\widehat{v}\|^2\right)^{1/2},$$

  where we take the Ritz value, respectively the Rayleigh quotient of the harmonic Ritz vector for (θ,η), and the refined vector $\widehat{u}\otimes\widehat{v}$.

TABLE 6.1
A comparison of the standard and harmonic extraction from three different subspaces for a right definite two-parameter eigenvalue problem.

	$b=50,\ d=0.02$ subspace = 3.6e-3		$b=40,\ d=0.03$ subspace = 4.0e-5		$b=50,\ d=0.03$ subspace = 4.2e-7	
	standard	harmonic	standard	harmonic	standard	harmonic
vector	1.9e-2	4.4e-3	3.7e-4	4.2e-5	1.6e-6	4.3e-7
value	1.2e-5	2.0e-2	1.2e-8	4.0e-5	2.5e-14	1.4e-8
residual	1.4e-1	1.8e-1	2.6e-3	4.2e-4	1.2e-5	3.0e-6
RQ value		4.6e-6		8.8e-9		1.5e-14
RQ residual		3.4e-2		3.9e-4		3.0e-6
refined vector	3.8e-3	3.8e-3	4.1e-5	4.1e-5	4.3e-7	4.3e-7
refined residual	3.1e-2	3.1e-2	3.9e-4	3.9e-4	3.0e-6	3.0e-6

From Table 6.1 we see that the harmonic extraction returns eigenvector approximations that are almost optimal, i.e., they are very close to the orthogonal projections of the exact

ETNA
Kent State University
etna@mcs.kent.edu

eigenvectors onto the search subspace. On the other hand, as is also usual for the standard eigenvalue problem, the harmonic Ritz values are less favorable approximations to the exact eigenvalues than the Ritz values. However, if we use the harmonic Ritz vector with its tensor Rayleigh quotient as approximation to the eigenvalue, we get better approximations and smaller residuals than in the standard extraction.

If we apply the refined extraction, where we take the Rayleigh quotient for the approximation of the eigenvalue, we can further improve the results. The improvement is substantial for the standard extraction but small for the harmonic extraction. Results after the refined extraction do not differ much, regardless whether we start with the standard or the harmonic extraction.

EXAMPLE 6.2. In the second example we take a random non right definite two-parameter eigenvalue problem of the same dimensions as in Example 6.1. Here we select the diagonal elements of F_1, F_2, G_1, G_2, H_1, and H_2 as complex numbers where both the real and the imaginary part are uniformly distributed random numbers from the interval $(-0.5, 0.5)$. Table 6.2 contains the results of similar numerical experiments as in Example 6.1.

TABLE 6.2
A comparison of the standard and harmonic extraction from three different subspaces for a non right definite two-parameter eigenvalue problem.

	$b = 50$, $d = 0.02$ subspace = 2.6e-3		$b = 40$, $d = 0.03$ subspace = 4.8e-5		$b = 50$, $d = 0.03$ subspace = 5.0e-7	
	standard	harmonic	standard	harmonic	standard	harmonic
vector	7.4e-3	2.6e-3	1.8e-4	4.9e-5	1.0e-5	5.1e-7
value	2.7e-3	1.5e-4	4.9e-5	4.7e-6	1.4e-6	4.1e-8
residual	1.8e-2	5.8e-3	4.5e-4	1.3e-4	2.9e-5	1.5e-6
RQ value		3.0e-3		3.8e-5		1.6e-6
RQ residual		7.5e-3		1.3e-4		3.1e-6
refined vector	2.6e-3	2.6e-3	4.9e-5	4.9e-5	5.1e-7	5.1e-7
refined residual	7.2e-3	7.5e-3	1.4e-4	1.3e-4	3.2e-6	3.1e-6

As in the previous example, the harmonic extraction returns almost optimal eigenvector approximations which are clearly better than the results of the standard extraction. Since this problem is non right definite, the error in the tensor Rayleigh quotient is linear in the eigenvector approximation error, compared to quadratic for the right definite problem in the previous example; see [11]. Again, we can improve the results using the refined extraction, in particular those of the standard extraction.

EXAMPLE 6.3. We take the right definite examples from Example 6.1 with density $d = 0.01$ and bandwidth $b = 80$. We compare the eigenvalues obtained by the Jacobi–Davidson method [11] where we apply the standard and harmonic extraction, respectively. We start with the same initial vectors and we test various numbers of inner GMRES steps for approximately solving the correction equation. We use the second order correction equation with the oblique projections, for the details see [11]. The maximum dimension of the search spaces is 14, after which we restart with three-dimensional spaces.

For the target (σ, τ) we take the arithmetic mean of the eigenvalues. In the extraction phase the standard or harmonic Ritz value is selected that is closest to a given target. Subsequently, we take the corresponding eigenvector approximation and take its tensor Rayleigh quotient as an approximate eigenvalue. As one can see in Examples 6.1 and 6.2, this gives a better approximation for the eigenvalue when we use the harmonic extraction, whereas it–naturally–does not change the eigenvalue approximation in the standard extraction.

We compute 100 eigenvalues, where we note that with a total number of 10^6 eigenvalues this problem cannot be considered a toy problem. The criterion for the convergence is that

ETNA
Kent State University
etna@mcs.kent.edu

the norm of the residual is below $5 \cdot 10^{-7}$. In the correction equation we use preconditioning with an incomplete LU factorization of the matrix $A_i - \sigma B_i - \tau C_i$ with a drop tolerance 10^{-3} for $i = 1, 2$.

If we use the standard extraction, then in each outer iteration the projected problem is right definite and we solve it using the algorithm in [24]. If we use the harmonic extraction, then the projected problem (3.4) is not definite. We could solve it with the method described in [10] using the QZ algorithm on (1.3), but experiments showed that we obtain very similar results by applying a cheaper but possibly unstable approach where we first solve one of the projected generalized eigenvalue problems (1.3) by solving the eigenvalue problem $\widetilde{\Delta}_0^{-1}\widetilde{\Delta}_1 z = \lambda z$, where $\widetilde{\Delta}_0$ and $\widetilde{\Delta}_1$ are the projected Δ_0 and Δ_1, and then insert the vector z in the second equation in order to obtain μ. All of the above methods require $\mathcal{O}(k^6)$ flops to solve the projected two-parameter eigenvalue problem, where k is the size of the search spaces.

The values in Table 6.3 are:

- *iter*: the number of outer iterations,
- *time*: time in seconds,
- *in 50, in 100*: the number of the computed eigenvalues that are among the 50 and 100 closest eigenvalues to the target, respectively.

TABLE 6.3
Comparison of the standard and harmonic extraction for the JD type method for a right definite two-parameter eigenvalue problem.

	Standard				Harmonic			
GMRES	iter	time	in 50	in 100	iter	time	in 50	in 100
4	2002	290	50	94	799	192	50	91
8	876	144	49	96	346	98	50	97
16	347	80	50	95	127	50	49	85
32	277	89	50	93	149	86	50	91
64	276	105	50	91	137	77	47	75

The results in Table 6.3 show that the harmonic extraction is faster and only slightly less accurate than the standard extraction. Solving the projected problems is more expensive for the harmonic extraction because they are not right definite, as opposed to the projected problems in the standard extraction. However, as the harmonic extraction requires far fewer outer iterations, it computes the eigenvalues faster than the standard extraction. On the other hand, the standard extraction returns a bit more accurate results, for instance, in all cases we get all 50 closest eigenvalues to the target. Both methods are suitable for this right definite two-parameter eigenvalue problem and based on the results we give the harmonic extraction a slight preference over the standard extraction.

We also applied the refined extraction, but in spite of the results in Tables 6.1 and 6.2, the experiments did not show advantages of the refined extraction. We do not report the results but we note that the refined method is more expensive and usually requires more outer iterations. As these remarks also apply to the remaining numerical examples in this section, we excluded the refined approach in the following.

As one can see in the next example, the difference between the standard and the harmonic extraction may be much more in favor of the harmonic extraction when we consider a non definite two-parameter eigenvalue problem.

EXAMPLE 6.4. In this example we take a random non right definite two-parameter eigenvalue problem with matrices of size 1000×1000 from Example 6.2 with density $d = 0.01$ and bandwidth $b = 80$. We perform similar experiments as in Example 6.3, the

ETNA
Kent State University
etna@mcs.kent.edu

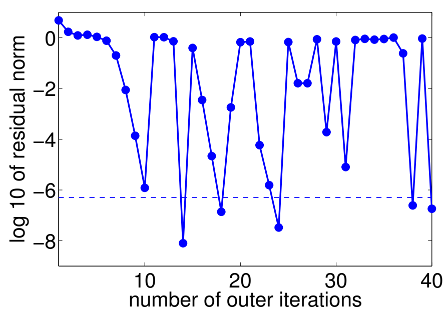
only difference is that now we use the two-sided Ritz extraction as well. As discussed in [10], this is a natural approach when we have a non definite two-parameter eigenvalue problem.

We limit the computation to 2500 outer iterations or to 50 extracted eigenvalues. Neither the one-sided standard nor the two-sided standard extraction is able to compute the required number of eigenvalues in the prescribed number of outer iterations (therefore, we omit the number of iterations and the cpu time for these methods). This is not an issue for the harmonic extraction which is a clear winner in this example. The results are presented in Table 6.4.

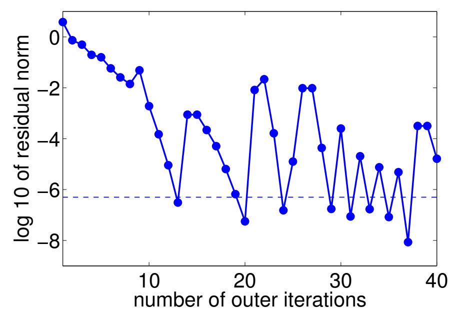
TABLE 6.4
Comparison of one-sided standard, two-sided standard, and harmonic extraction methods for the JD type method for a non right definite two-parameter eigenvalue problem.

	One-sided standard			Two-sided standard			Harmonic				
GMRES	eigs	in 10	in 30	eigs	in 10	in 30	iter	time	in 10	in 30	in 50
4	9	9	9	8	8	8	594	272	10	30	47
8	17	10	17	12	9	12	226	119	10	30	46
16	19	10	19	19	10	19	106	73	10	30	44
32	20	10	20	22	10	22	89	87	10	29	40
64	22	10	22	30	10	29	93	118	10	28	40

Figure 6.1 shows the convergence graphs for the two-sided extraction (a) and the harmonic extraction (b) for the first 40 outer iterations, in both cases we take 8 GMRES steps in the inner iteration. One can see that the convergence is more erratic when we use the standard extraction and smoother (almost monotonous) if we use the harmonic extraction.



(a)



(b)

FIG. 6.1. *Comparison of convergence using the two-sided Ritz extraction (a) and the harmonic extraction (b).*

EXAMPLE 6.5. Using the same non right definite problem as in Example 6.3 we test how many eigenvalues can we extract with a limited number of matrix-vector multiplications, i.e., we fix the product of inner and outer iterations. The limit is 3200.

TABLE 6.5
Eigenvalues obtained using the harmonic extraction and 3200 inner iterations.

GMRES	all	in 25	in 50	time (sec)
4	59	25	50	358
8	68	25	50	213
16	75	25	49	141
32	52	24	40	97
64	24	18	21	58

The results in Table 6.5 show that for a low number of inner iterations we get fewer eigenvalues and spend more time, but the possibility to compute an unwanted eigenvalue is smaller. If we use more inner iterations we get many unwanted eigenvalues, but spend less time. The optimal combination is to take a moderate number of inner iterations, in this example this would be between 16 and 32 inner steps.

Besides the matrix-vector multiplications, the most time consuming operation is to solve the projected low-dimensional two-parameter eigenvalue problem in each outer step. If the search spaces are of size k, then we need $\mathcal{O}(k^6)$ flops to solve these projected problems. Since this is relatively expensive compared to the work for the matrix-vector multiplications, it is a good idea to use several GMRES steps (but not too many to avoid convergence to an unwanted eigenvalue) to try to reduce the number of outer iterations.

EXAMPLE 6.6. In this example we take a non right definite two-parameter eigenvalue problem where A_i, B_i, and C_i are random complex banded matrices of size 500×500 generated by the Matlab command

```
M=sparse(triu(tril(randn(500)+i*randn(500),5),-5));
```

where M is respectively equal to A_1, B_1, C_1, A_2, B_2, and C_2.

TABLE 6.6
Comparison of standard and harmonic extraction for a non right definite two-parameter eigenvalue problem.

	One-sided standard			Two-sided standard			Harmonic			
GMRES	eigs	time	in 5	eigs	time	in 5	iter	time	in 5	in 10
4	0	347	0	3	463	3	683	253	5	10
8	0	417	0	3	559	3	730	308	5	8
16	0	544	0	4	791	3	244	134	5	7
32	1	626	1	3	1204	4	343	280	5	8
64	1	668	1	3	1286	3	515	255	5	8

We look for the eigenvalues closest to the origin and for a preconditioner we take $M_i = A_i$ for $i = 1, 2$. We limit the computation to 1000 outer iteration or 15 extracted eigenvalues.

From the results in Table 6.6 one can see clearly that the harmonic extraction extracts more eigenvalues than the standard extraction. Both the one-sided and the two-sided standard Ritz extraction fail to compute 15 eigenvalues in 1000 outer iterations; therefore, the number of iterations is displayed only for the harmonic extraction, the number of iterations for both the one-sided and two-sided Ritz extraction is 1000. The one-sided standard extraction is particularly poor in view of the fact that it manages to compute at most one eigenvalue. The two-sided Ritz extraction computes more eigenvalues, but falls considerably short of the required 15. For this example the harmonic extraction is clearly the suggested method.

EXAMPLE 6.7. We take the two-parameter eigenvalue problem from Example 8.4 in [10]. The problem is non right definite and the matrices are of size 1000×1000. We used this problem in [10] to demonstrate that the two-sided Ritz extraction may give better results than the one-sided standard extraction. We limit the computation to 500 outer iterations or 30 extracted eigenvalues. For the target we take the arithmetic mean of the eigenvalues.

The results in Table 6.7 show that the harmonic extraction is a substantial improvement to the standard extraction. As in the previous example, both the one-sided and two-sided Ritz extraction fail to compute the required number of eigenvalues in the available number of outer iterations. The number of iterations is displayed in Table 6.7 only for the harmonic extraction, the number of iterations for one-sided and two-sided Ritz extraction is 500.

7. Conclusions. It was observed in [11] that the multiparameter eigenvalue problem is a challenge, especially with respect to the task of finding interior eigenvalues. The concept of a harmonic extraction technique for the MEP was left as an open question, and dealt with in

ETNA
Kent State University
etna@mcs.kent.edu

TABLE 6.7
Comparison of standard and harmonic extraction for a non right definite two-parameter eigenvalue problem.

	One-sided standard			Two-sided standard			Harmonic			
GMRES	eigs	time	in 10	eigs	time	in 10	iter	time	in 10	in 20
10	11	671	4	15	1041	6	116	282	10	17
20	11	948	4	21	1542	9	95	308	10	18
30	10	1146	3	20	2062	8	110	400	10	19

this paper. We have seen that, although there seems to be no straightforward generalization of a spectral transformation (2.1) for the MEP, the harmonic approach can be generalized to the MEP, with a corresponding elegant and intuitive generalization of Saad's theorem. We also gave a generalization of the refined extraction, which seems to be less suited for this problem.

Based on the theory and the numerical results, our recommendations for the numerical computation of interior eigenvalues of a MEP are the following. For right definite MEPs we use the one-sided Jacobi–Davidson method [11] for the subspace expansion. The harmonic extraction presented in this paper is at least very competitive with the standard extraction described in [11]. For non right definite problems, the one-sided approach [11] combined with the harmonic extraction, described in this paper, is both faster and more accurate than the two-sided approach proposed in [10], which on its turn is more accurate than the one-sided approach with standard extraction [11].

For exterior eigenvalues we opt for the standard extraction, combined with a one-sided approach for right definite MEPs [11], or a two-sided approach for non right definite MEPs [10].

It is important to realize that for the MEP solving the projected problems is itself already a computationally non-negligible task in view of the $\mathcal{O}(k^6)$ costs. Therefore it is advisable to invest in solving the correction equations relatively accurately to minimize these costs. Hence, although just a few steps of GMRES may give more accurate results because we compute fewer unwanted eigenpairs, this may be much more time demanding.

Finally, we remark that a two-sided harmonic approach is possible, but much less effective since the correspondence between right and left approximate eigenvectors is lost; we will not go into further details. The methods in this paper can be generalized to MEPs with more than two parameters in a straightforward way; see, e.g., [12] for some more details on these MEPs. MATLAB code of the methods is available on request.

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