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Minimization principles and computation for the generalized linear response eigenvalue problem

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Abstract The minimization principle and Cauchy-like interlacing inequalities for the generalized linear response eigenvalue problem are presented. Based on these theoretical results, the best approximations through structure-preserving subspace projection and a locally optimal block conjugate gradient-like algorithm for simultaneously computing the first few smallest eigenvalues with the positive sign are proposed. Numerical results are presented to illustrate essential convergence behaviors of the proposed algorithm.

Keywords Eigenvalue · Eigenvector · Minimization principle · Conjugate gradient · Linear response

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Dedicated to Professor Axel Ruhe on the occasion of his 70th birthday.

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1 Introduction

In [2,3,19,21], minimization principles and locally optimal 4-D conjugate gradient methods are established for the eigenvalue problem of the form:

$$\begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix}, \tag{1.1}$$

where K and M are $n \times n$ real symmetric positive semi-definite matrices and one of them is definite. It is referred to as the *linear response* (*LR*) *eigenvalue problem* because it is equivalent to the eigenvalue problem

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \lambda \begin{bmatrix} u \\ v \end{bmatrix} \tag{1.2}$$

via a similarity transformation with the orthogonal matrix

$$J = \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & I_n \\ I_n & -I_n \end{bmatrix}, \tag{1.3}$$

where A and B are $n \times n$ real symmetric matrices such that the symmetric matrix $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ is symmetric positive definite[1]. The eigenvalue problem (1.2) is the computational kernel in the response theory models for analyzing the response of a self-consistent-field state to an external perturbation in computational physics and chemistry, e.g., see [9,14,16,20]. The eigenvalue problem (1.2) is also widely known as a random phase approximation eigenvalue problem, e.g. see [17,18].

The generalized LR eigenvalue problem is of the form

$$\begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \lambda \begin{bmatrix} \Sigma & \Delta \\ \Delta & \Sigma \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}, \tag{1.4}$$

where A and B are as in (1.2), and Σ and Δ are also $n \times n$ with Σ being symmetric while Δ skew-symmetric (i.e., $\Delta^{\mathrm{T}} = -\Delta$) such that $\begin{bmatrix} \Sigma & \Delta \\ \Delta & \Sigma \end{bmatrix}$ is nonsingular. The generalized eigenvalue problem (1.4) arises from the study of transition properties and second and higher order response properties using a response function approach [7,14,15].

The generalized LR eigenvalue problem (1.4) can be transformed via the orthogonal matrix J to an equivalent eigenvalue problem that differs from (1.1) in the right hand side. In fact, it is easy to verify that

$$J^{\mathrm{T}} \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} J J^{\mathrm{T}} \begin{bmatrix} u \\ v \end{bmatrix} = \lambda J^{\mathrm{T}} \begin{bmatrix} \Sigma & \Delta \\ \Delta & \Sigma \end{bmatrix} J J^{\mathrm{T}} \begin{bmatrix} u \\ v \end{bmatrix}$$

[1] This condition is equivalent to that both $A \pm B$ are positive definite. In [2,3] and this article, we focus on very much this case, except that one of $A \pm B$ is allowed to be positive semi-definite.

gives rise to

$$Hz \equiv \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} E_+ & 0 \\ 0 & E_- \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} \equiv \lambda E z, \tag{1.5}$$

where

$$K = A - B,\ M = A + B,\ E_{\pm} = \Sigma \pm \Delta, \ \text{ and } \begin{bmatrix} y \\ x \end{bmatrix} = J^{\mathrm{T}} \begin{bmatrix} u \\ v \end{bmatrix}. \tag{1.6}$$

Furthermore, the positive definiteness of $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ and the nonsingularity of $\begin{bmatrix} \Sigma & \Delta \\ \Delta & \Sigma \end{bmatrix}$ are equivalent to that both K and M are positive definite, and $E_{\pm}$ are nonsingular[2]. Hence the eigenvalue problems (1.4) and (1.5) are equivalent: both have the same eigenvalues with corresponding eigenvectors related by

$$\begin{bmatrix} u \\ v \end{bmatrix} = J \begin{bmatrix} y \\ x \end{bmatrix}. \tag{1.7}$$

The imposed conditions on A, B, Σ, and Δ imply that *both K and M are real symmetric positive definite and $E_{\pm}$ are nonsingular and $E_+^{\mathrm{T}} = E_-$*. In the rest of this article, the condition on K and M will be relaxed to that *both are symmetric positive semi-definite and one of them is definite*, unless explicitly stated otherwise.

Later, we will see that the $2n$ eigenvalues of (1.5) are all real:

$$-\lambda_n \le \cdots \le -\lambda_1 \le +\lambda_1 \le \cdots \le +\lambda_n.$$

Our main contributions in this paper are as follows.

1. As an extension of Thouless' minimization principle, we will prove

$$\lambda_1 = \inf_{x,y} \frac{x^{\mathrm{T}} K x + y^{\mathrm{T}} M y}{2|x^{\mathrm{T}} E_+ y|}. \tag{1.8}$$

   In the case when $E_{\pm} = I$ and both K and M are definite, (1.8) becomes Thouless' minimization principle [19,21,2].
2. We will prove a subspace version of the minimization principle (1.8):

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf_{\substack{U^{\mathrm{T}} E_+ V = I_k \\ U, V \in \mathbb{R}^{n \times k}}} \operatorname{trace}(U^{\mathrm{T}} K U + V^{\mathrm{T}} M V). \tag{1.9}$$

   In the case when $E_{\pm} = I$, (1.9) has already been proven in [2].

[2] It suffices to assume one of $E_{\pm}$ is nonsingular since $E_{\pm}^{\mathrm{T}} = E_{\mp}$.

3. Let U and V be $n \times \ell$ (where $\ell < n$) such that $W \stackrel{\rm def}{=} U^{\rm T} E_+ V$ is nonsingular, and factorize W as $W = W_1^{\rm T} W_2$, where W_i are $\ell \times \ell$ (and thus necessarily nonsingular). Define

$$H_{\rm SR} = \begin{bmatrix} 0 & W_1^{-\rm T} U^{\rm T} K U W_1^{-1} \\ W_2^{-\rm T} V^{\rm T} M V W_2^{-1} & 0 \end{bmatrix} \tag{1.10}$$

and denote the eigenvalues of $H_{\rm SR}$ by $-\mu_\ell \le \cdots \le -\mu_1 \le +\mu_1 \le \cdots \le +\mu_\ell$. We obtain Cauchy-like inequalities for λ_i and μ_i (see Theorem 3.4). In addition, we also show that

$$\sum_{i=1}^{k} \mu_i = \frac{1}{2} \inf_{\substack{\widehat{U}^{\rm T} E_+ \widehat{V} = I_k \\ {\rm span}(\widehat{U}) \subseteq \mathcal{U},\ {\rm span}(\widehat{V}) \subseteq \mathcal{V}}} {\rm trace}(\widehat{U}^{\rm T} K \widehat{U} + \widehat{V}^{\rm T} M \widehat{V}), \tag{1.11}$$

where $\mathcal{U} = {\rm span}(U)$ and $\mathcal{V} = {\rm span}(V)$ are the column spaces of U and V, respectively.
4. Combining (1.10) and (1.11) with a variation of the classical conjugate gradient method, we establish a locally optimal block 4-D preconditioned conjugate gradient method to simultaneously compute the several smallest eigenvalues with the positive sign of the generalized LR eigenvalue problem (1.5).

The rest of this paper is organized as follows. In Sect. 2, we review basic theoretical results about the eigenvalue problem (1.1) and then introduce the concept of a pair of deflating subspaces and its approximation properties. In Sect. 3, we will prove a couple of the minimization principles and Cauchy-like interlacing inequalities. In Sect. 4, we discuss the metric about the best approximation from a pair of approximate deflating subspaces. In Sect. 5, we apply newly established minimization principles to derive CG type algorithms for computing the first few λ_i. In Sect. 6, we present numerical results to illustrate the convergence behaviors of CG methods. Concluding remarks are in Sect. 7.

2 Basic theory and pair of deflating subspaces

2.1 Basics

In this subsection, we discuss some basic theoretical results on the LR eigenvalue problem (1.5). Mehl et al. [11] investigated the canonical forms of the same eigenvalue problem (1.5) under a more general context, namely no assumptions on K and M being positive (semi-)definite, except symmetry, and $E_\pm$ being nonsingular. The results below in this section can essentially be derived from their more general setting, but in our context they can also be easily derived (see [1] for details). For this reason, we will leave out the proofs of the theorems in this subsection.

Decompose $E_\pm$ as

$$E_-^{\rm T} = E_+ = C D^{\rm T}, \tag{2.1}$$

where $C,\ D \in \mathbb{R}^{n \times n}$ are nonsingular. How this factorization is done is not mathematically essential. For example, we can simply let one of C and D be I_n.

With (2.1), the LR eigenvalue problem (1.5) is equivalent to

$$\mathcal{H}w \equiv \begin{bmatrix} 0 & \mathcal{K} \\ \mathcal{M} & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix}, \tag{2.2}$$

where

$$\mathcal{K} = C^{-1}KC^{-\mathrm{T}},\ \mathcal{M} = D^{-1}MD^{-\mathrm{T}},\ \begin{bmatrix} y \\ x \end{bmatrix} = \Gamma^{\mathrm{T}} \begin{bmatrix} y \\ x \end{bmatrix},\ \text{and}\ \Gamma = \begin{bmatrix} D & \\ & C \end{bmatrix}. \tag{2.3}$$

We now have two equivalent eigenvalue problems (1.5) and (2.2) in the sense that both have the same eigenvalues and their eigenvectors are related by the relation shown in (2.3).

The problem (2.2) takes the same form as (1.1), making it possible for us to simply adapt the results in [2,3] for (2.2) and then translate them for the generalized LR eigenvalue problem (1.5). However, we should note that for practical considerations, the problem (2.2) should never be explicitly formed to avoid destroying. e.g., the sparsity in K and M or other structural properties. Sometimes K, M, and $E_\pm$ simply may not be available and their very existences are through matrix-vector multiplications. In such cases, explicitly forming (2.2) just cannot be accomplished. For our purpose in this paper, the significance of transforming (1.5) into (2.2) lies only in theoretical developments and efficient algorithm derivations.

For the eigenvalue problem (2.2), we know that $\mathcal{K}$, $\mathcal{M} \succeq 0$ because K, $M \succeq 0$, where $X \succ 0$ ($X \succeq 0$) means X is real symmetric positive (semi-)definite. As argued in [2] for (1.1), the eigenvalues for (2.2) are real and come in $\pm\lambda$ pairs. More precisely, denote the eigenvalues of $\mathcal{K}\mathcal{M}$ by λ_i^2 ($1 \le i \le n$) in the ascending order:

$$0 \le \lambda_1^2 \le \lambda_2^2 \le \cdots \le \lambda_n^2, \tag{2.4}$$

where all $\lambda_i \ge 0$ and thus $0 \le \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. The eigenvalues of $\mathcal{M}\mathcal{K}$ are λ_i^2 ($1 \le i \le n$), too. The eigenvalues of $H - \lambda E$ are then $\pm\lambda_i$ for $i = 1, 2, \ldots, n$ with the ordering

$$-\lambda_n \le \cdots \le -\lambda_1 \le +\lambda_1 \le \cdots \le +\lambda_n. \tag{2.5}$$

For convenience, we shall associate half of 0 eigenvalues with the positive sign and the other half with the negative sign, as argued in [2]. Doing so legitimizes the use of the phrase “the first k smallest eigenvalues with the positive sign of $H - \lambda E$” to refer to λ_i for $1 \le i \le k$ without ambiguity even when $\lambda_1 = +0$. Throughout this paper, we will stick to using $\pm\lambda_i$ for $1 \le i \le n$ in the order of (2.5) to denote the eigenvalues of $H - \lambda E$.

Set

$$\mathscr{I} = \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix}, \quad \mathscr{I}_E = \begin{bmatrix} 0 & E_- \\ E_+ & 0 \end{bmatrix} = \Gamma \mathscr{I} \Gamma^{\mathrm{T}}, \tag{2.6}$$

where Γ is given in (2.3). Both are symmetric but indefinite. The matrices $\mathscr{I}_E$ and $\mathscr{I}$ induce *indefinite inner products* on $\mathbb{R}^{2n}$:

$$\langle z_1, z_2 \rangle_{\mathscr{I}_E} \stackrel{\text{def}}{=} z_1^{\mathrm{T}} \mathscr{I}_E z_2 \equiv \langle w_1, w_2 \rangle_{\mathscr{I}} \stackrel{\text{def}}{=} w_1^{\mathrm{T}} \mathscr{I} w_2,$$

where $w_i = \Gamma^{\mathrm{T}} z_i$. The following theorem tells us some orthogonality properties among the eigenvectors for $H - \lambda E$.

Theorem 2.1 1. *Let (α, z) be an eigenpair of $H - \lambda E$, where $z = \begin{bmatrix} y \\ x \end{bmatrix} \neq 0$ and $x,\ y \in \mathbb{R}^n$. Then $\alpha \langle z, z \rangle_{\mathscr{I}_E} = 2\alpha\, x^{\mathrm{T}} E_+ y > 0$ if $\alpha \neq 0$. In particular, this implies $\langle z, z \rangle_{\mathscr{I}_E} = 2x^{\mathrm{T}} E_+ y \neq 0$ if $\alpha \neq 0$.*

2. *Let (α_i, z_i) $(i = 1, 2)$ be two eigenpairs of $H - \lambda E$. Partition $z_i = \begin{bmatrix} y_i \\ x_i \end{bmatrix} \neq 0$, where $x_i,\ y_i \in \mathbb{R}^n$.*
   a. *If $\alpha_1 \neq \alpha_2$, then $\langle z_1, z_2 \rangle_{\mathscr{I}_E} = y_1^{\mathrm{T}} E_- x_2 + x_1^{\mathrm{T}} E_+ y_2 = 0$.*
   b. *If $\alpha_1 \neq \pm\alpha_2 \neq 0$, then $y_1^{\mathrm{T}} E_- x_2 = x_1^{\mathrm{T}} E_+ y_2 = 0$.*

For the sake of presentation, in what follows we either assume that M is definite or only provide proofs for definite M whenever one of K and M is required to be definite. Doing so loses no generality because the interchangeable roles played by K and M make it rather straightforward to create a version for the case when K is definite by simply swapping K and M in each of their appearances and E_+ and E_- in each of their appearances.

Theorem 2.2 *Suppose that $M \succ 0$, and define C and D by (2.1). Then the following statements are true:*

1. *There exist nonsingular $\mathcal{X},\ \mathcal{Y} \in \mathbb{R}^{n \times n}$ such that*

$$K = C\mathcal{Y}\Lambda^2\mathcal{Y}^{\mathrm{T}}C^{\mathrm{T}}, \quad M = D\mathcal{X}\mathcal{X}^{\mathrm{T}}D^{\mathrm{T}}, \tag{2.7}$$

   where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $\mathcal{X} = \mathcal{Y}^{-\mathrm{T}}$.
2. *If K is also definite, then all $\lambda_i > 0$ and $H - \lambda E$ is diagonalizable:*

$$HZ = EZ \begin{bmatrix} \Lambda & \\ & -\Lambda \end{bmatrix}, \quad \text{where} \quad Z = \Gamma^{-\mathrm{T}} \begin{bmatrix} \mathcal{Y}\Lambda & \mathcal{Y}\Lambda \\ \mathcal{X} & -\mathcal{X} \end{bmatrix}. \tag{2.8}$$

3. *$H - \lambda E$ is not diagonalizable if and only if $\lambda_1 = 0$ which happens when and only when K is singular.*
4. *The ith column of Z is the eigenvector of $H - \lambda E$ corresponding to λ_i, where $1 \le i \le n$, and it is unique if*
   a. *λ_i is a simple eigenvalue of (2.2), or*
   b. *$i = 1, \lambda_1 = +0 < \lambda_2$. In this case, 0 is a double eigenvalue of $H - \lambda E$ but there is only one eigenvector associated with it.*

5. *If* $0 = \lambda_1 = \cdots = \lambda_\ell < \lambda_{\ell+1}$, *then the Kronecker canonical form of* $H - \lambda E$ *is*

$$\underbrace{\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}}_{\ell} \oplus \operatorname{diag}(\lambda_{\ell+1}, -\lambda_{\ell+1}, \ldots, \lambda_n, -\lambda_n) - \lambda I_{2n}, . \tag{2.9}$$

where $X_1 \oplus \cdots \oplus X_k$ *denote a block-diagonal matrix with* i*th diagonal block* X_i. *Thus* $H - \lambda E$ *has* 0 *as an eigenvalue of algebraic multiplicity* 2ℓ *with only* ℓ *linearly independent eigenvectors which are the columns of* $\Gamma^{-\mathrm{T}} \begin{bmatrix} 0 \\ \mathcal{X}_{(:,1:\ell)} \end{bmatrix}$.

2.2 Pair of deflating subspaces

Let $\mathcal{U}, \mathcal{V} \subseteq \mathbb{R}^n$ be subspaces. We call $\{\mathcal{U}, \mathcal{V}\}$ a *pair of deflating subspaces* of $H - \lambda E$ if

$$K\mathcal{U} \subseteq E_+\mathcal{V} \quad \text{and} \quad M\mathcal{V} \subseteq E_-\mathcal{U}. \tag{2.10}$$

Let $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times \ell}$ be the basis matrices for the subspaces $\mathcal{U}$ and $\mathcal{V}$, respectively, where $\dim(\mathcal{U}) = k$ and $\dim(\mathcal{V}) = \ell$. Then (2.10) implies that there exist $K_{\mathrm{R}} \in \mathbb{R}^{\ell\times k}$ and $M_{\mathrm{R}} \in \mathbb{R}^{k\times \ell}$ such that

$$KU = E_+VK_{\mathrm{R}}, \quad MV = E_-UM_{\mathrm{R}}. \tag{2.11}$$

Given U and V, both K_{R} and M_{R} are uniquely determined by respective equations in (2.11), but there are numerous ways to express them. In fact for any left generalized inverses $U^{\dashv}$ and $V^{\dashv}$ of E_-U and E_+V, respectively, i.e., $U^{\dashv}E_-U = I_k$ and $V^{\dashv}E_+V = I_\ell$,

$$K_{\mathrm{R}} = V^{\dashv}KU, \quad M_{\mathrm{R}} = U^{\dashv}MV. \tag{2.12}$$

There are infinitely many left generalized inverses $U^{\dashv}$ and $V^{\dashv}$. For example,

$$U^{\dashv} = (U^{\mathrm{T}}E_-U)^{-1}U^{\mathrm{T}} \quad \text{if } (U^{\mathrm{T}}E_-U)^{-1}\text{exists},$$
$$V^{\dashv} = (V^{\mathrm{T}}E_+V)^{-1}V^{\mathrm{T}} \quad \text{if } (V^{\mathrm{T}}E_+V)^{-1}\text{exists}$$

or, if $U^{\mathrm{T}}E_+V = (V^{\mathrm{T}}E_-U)^{\mathrm{T}}$ is nonsingular, then

$$U^{\dashv} = (V^{\mathrm{T}}E_-U)^{-1}V^{\mathrm{T}}, \quad V^{\dashv} = (U^{\mathrm{T}}E_+V)^{-1}U^{\mathrm{T}}. \tag{2.13}$$

But still K_{R} and M_{R} are unique. The left generalized inverses in (2.13) will become important later in preserving symmetry in K and M.

Define

$$H_{\mathrm{R}} = \begin{bmatrix} 0 & K_{\mathrm{R}} \\ M_{\mathrm{R}} & 0 \end{bmatrix}. \tag{2.14}$$

Then H_{R} is the restriction of $H - \lambda E$ onto $\mathcal{V} \oplus \mathcal{U}$ with respect to the basis matrix $V \oplus U$:

$$H \begin{bmatrix} V & \\ & U \end{bmatrix} = E \begin{bmatrix} V & \\ & U \end{bmatrix} H_{\mathrm{R}}. \tag{2.15}$$

H_{R} in (2.14) inherits the block structure in H: zero blocks remain zero blocks. But when K and M are symmetric, in general H_{R} may lose the symmetry property in its off-diagonal blocks K_{R} and M_{R}, not to mention positive semi-definiteness in K and M. We propose a modification to H_{R} to overcome this potential loss, when

$$W \overset{\text{def}}{=} U^{\mathrm{T}} E_{+} V$$

is nonsingular. Factorize $W = W_1^{\mathrm{T}} W_2$, where W_1 and W_2 are nonsingular, and define

$$H_{\mathrm{SR}} = \begin{bmatrix} 0 & W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1} \\ W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1} & 0 \end{bmatrix}. \tag{2.16}$$

Note H_{SR} shares not only the block structure in H but also the symmetry and semi-definiteness in its off-diagonal blocks.

Theorem 2.3 *Let H_{SR} be defined by (2.16). Then*

$$H \begin{bmatrix} V W_2^{-1} & \\ & U W_1^{-1} \end{bmatrix} = E \begin{bmatrix} V W_2^{-1} & \\ & U W_1^{-1} \end{bmatrix} H_{SR}. \tag{2.17}$$

Consequently, if $(\hat{\lambda}, \hat{z})$ is an eigenpair of H_{SR}, then $z = \begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} V W_2^{-1} \hat{y} \\ U W_1^{-1} \hat{x} \end{bmatrix}$ is an eigenpair of the LR eigenproblem $H - \lambda E$, where $\hat{z} = \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix}$ is conformally partitioned.

Proof Equations in (2.11) hold for some K_{R} and M_{R}. Thus

$$U^{\mathrm{T}} K U = (U^{\mathrm{T}} E_{+} V) K_{\mathrm{R}} = W_1^{\mathrm{T}} W_2 K_{\mathrm{R}},$$
$$V^{\mathrm{T}} M V = (V^{\mathrm{T}} E_{-} U) M_{\mathrm{R}} = W_2^{\mathrm{T}} W_1 M_{\mathrm{R}},$$

which gives

$$W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1} = W_2 K_{\mathrm{R}} W_1^{-1}, \quad W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1} = W_1 M_{\mathrm{R}} W_2^{-1}. \tag{2.18}$$

Now use (2.11) and (2.18) to get

$$\begin{aligned} K(U W_1^{-1}) &= E_{+} V K_{\mathrm{R}} W_1^{-1} \\ &= E_{+}(V W_2^{-1})(W_2 K_{\mathrm{R}} W_1^{-1}) \\ &= E_{+}(V W_2^{-1})(W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1}), \\ M(V W_2^{-1}) &= E_{-}(U W_1^{-1})(W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1}). \end{aligned}$$

They yield (2.17).

Multiply $\hat{z}$ to the both sides of (2.17) from the right and use $H_{\mathrm{SR}} \hat{z} = \hat{\lambda} \hat{z}$ to conclude the rest of the theorem. □

Note that the well-definedness of H_{SR} as in (2.16) alone does not require $\{\mathrm{span}(U), \mathrm{span}(V)\}$ be a pair of deflating subspaces of $H - \lambda E$. For that, the nonsingularity of $U^{\mathrm{T}} E_+ V$ is sufficient. H_{SR} will play particularly important roles in the rest of this article.

2.3 Approximate pair of deflating subspaces

In practical computations, rarely pairs of exact deflating subspaces are known, only approximate ones. The question then arises: how to compute approximate eigenpairs of $H - \lambda E$ given a pair of *approximate* deflating subspaces. Theorem 2.3 shed light on how this can be done.

Let $\{\mathcal{U}, \mathcal{V}\}$ be a pair of *approximate* deflating subspaces. Pick basis matrices U and V of $\mathcal{U}$ and $\mathcal{V}$, respectively, and define H_{SR} according to (2.16). The following algorithm returns approximate eigenvalues and eigenvectors of $H - \lambda E$ from the given approximate pair of deflating subspaces $\{\mathcal{U}, \mathcal{V}\}$:

Algorithm 2.1 1. Construct H_{SR} as in (2.16) if $U^{\mathrm{T}} E_+ V$ is nonsingular;
2. Compute the eigenpairs $\left\{\hat{\lambda}, \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix}\right\}$ of H_{SR};
3. The computed eigenvalues $\hat{\lambda}$ approximate some eigenvalues of $H - \lambda E$, and the associated approximate eigenvectors are $\begin{bmatrix} V W_2^{-1} \hat{y} \\ U W_1^{-1} \hat{x} \end{bmatrix}$ according to Theorem 2.3.

Given two subspaces $\mathcal{U}$ and $\mathcal{V}$, there are many ways to construct H_{SR} due to the factorization $W = W_1^{\mathrm{T}} W_2$ and basis matrices U and V are not unique. The argument similar to the one in [3] can be used to argue that the approximations by Algorithm 2.1 are invariant with respect to how H_{SR} is constructed. See also [1].

3 Minimization principles

Define the functional

$$\rho(x, y) \stackrel{\mathrm{def}}{=} \frac{x^{\mathrm{T}} K x + y^{\mathrm{T}} M y}{2|x^{\mathrm{T}} E_+ y|}, \tag{3.1}$$

where $y^{\mathrm{T}} E_- x$ can be used in place of $x^{\mathrm{T}} E_+ y$ due to the fact $(x^{\mathrm{T}} E_+ y)^{\mathrm{T}} = y^{\mathrm{T}} E_- x$ for any x and y. Relating (1.5) to (1.4) through the transformation (1.7), we find

$$\rho(x, y) \equiv \varrho(u, v) \stackrel{\mathrm{def}}{=} \frac{\begin{bmatrix} u \\ v \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} A & B \\ B & A \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}}{\left| \begin{bmatrix} u \\ v \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \Sigma & \Delta \\ -\Delta & -\Sigma \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \right|}. \tag{3.2}$$

Both $\varrho(u, v)$ and $\rho(x, y)$ were defined in [2] but only for the case $E_\pm = I_n$ and, correspondingly, $\Sigma = I_n$ and $\Delta = 0$. We will call them, without distinction, the *Thouless functional* (in different forms).

Several theoretical results for the case $E = I_{2n}$ were established in [2]. In this section, we establish analogs of these results for the matrix pencil $H - \lambda E$.

3.1 Minimization principles

Theorem 3.1 is actually a corollary of Theorem 3.2, it is presented here for its simplicity.

Theorem 3.1 *We have*

$$\lambda_1 = \inf_{x,y} \rho(x, y). \tag{3.3}$$

Moreover, "$\inf$*" can be replaced by "*$\min$*" if and only if both* $K, M \succ 0$. *When both* $K, M \succ 0$, *the optimal argument pair* (x, y) *gives rise to an eigenvector* $z = \begin{bmatrix} y \\ x \end{bmatrix}$ *of* $H - \lambda E$ *associated with* λ_1.

Proof It is easy to see that

$$\rho(x, y) = \frac{\chi^{\mathrm{T}} \mathcal{K} \chi + y^{\mathrm{T}} \mathcal{M} y}{2|\chi^{\mathrm{T}} y|},$$

where $\chi = C^{\mathrm{T}} x$, $y = D^{\mathrm{T}} y$, and $\mathcal{K}$ and $\mathcal{M}$ are as given in (2.3). The theorem is then a consequence of [2, Theorem 3.1]. □

Owing to that (1.5) and (1.4) being equivalent through the transformation (1.7), we have for the original LR problem (1.4)

$$\lambda_1 = \inf_{u,v} \varrho(u, v). \tag{3.4}$$

For the case $\Sigma = I_n$ and $\Delta = 0$ and when both $K, M \succ 0$, this was established by Thouless [19].

Theorem 3.2 *We have*

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf_{\substack{U^{\mathrm{T}} E_+ V = I_k \\ U, V \in \mathbb{R}^{n \times k}}} \operatorname{trace}(U^{\mathrm{T}} K U + V^{\mathrm{T}} M V). \tag{3.5}$$

Moreover, "$\inf$*" can be replaced by "*$\min$*" if and only if both* $K, M \succ 0$. *When both* $K, M \succ 0$ *and if also* $\lambda_k < \lambda_{k+1}$, *then for any* U *and* V *that attain the minimum,* $\{\operatorname{span}(U), \operatorname{span}(V)\}$ *is a pair of deflating subspaces of* $H - \lambda E$ *and the corresponding* H_{SR} *has eigenvalues* $\pm\lambda_i$ *for* $1 \le i \le k$.

Proof We notice that

$$U^{\mathrm{T}} K U + V^{\mathrm{T}} M V = \mathcal{U}^{\mathrm{T}} \mathcal{K} \mathcal{U} + \mathcal{V}^{\mathrm{T}} \mathcal{M} \mathcal{V}, \; U^{\mathrm{T}} E_+ V = \mathcal{U}^{\mathrm{T}} \mathcal{V},$$

where $\mathcal{U} = C^{\mathrm{T}}U$ and $\mathcal{V} = D^{\mathrm{T}}V$. Therefore, the theorem is a consequence of [2, Theorem 3.2], □

Exploiting the close relation (3.2) between the two different functionals $\varrho(\cdot,\cdot)$ and $\rho(\cdot,\cdot)$, we have by Theorem 3.2 the following theorem for the original LR eigenvalue problem (1.4).

Theorem 3.3 *Suppose that $A,\ B,\ \Sigma \in \mathbb{R}^{n\times n}$ are symmetric and $\Delta \in \mathbb{R}^{n\times n}$ is anti-symmetric, and that both $A \pm B \succeq 0$ and one of them is definite and $\Sigma \pm \Delta$ are nonsingular. Then we have*

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf \operatorname{trace}\left(\begin{bmatrix} U \\ V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} A & B \\ B & A \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix}\right), \tag{3.6}$$

where "inf" *is taken over all $U,\ V \in \mathbb{R}^{n\times k}$ subject to*

$$\begin{bmatrix} U \\ V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \Sigma & \Delta \\ -\Delta & -\Sigma \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix} = 2I_k \quad \text{and} \quad \begin{bmatrix} U \\ V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} \Sigma & \Delta \\ -\Delta & -\Sigma \end{bmatrix} \begin{bmatrix} V \\ U \end{bmatrix} = 0. \tag{3.7}$$

Moreover, "inf" *can be replaced by* "min" *if and only if both $A \pm B \succ 0$.*

Proof Assume the assignments in (1.6) for K and M. We have

$$\begin{bmatrix} U \\ V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} A & B \\ B & A \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix} = \begin{bmatrix} \widehat{V} \\ \widehat{U} \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} M & \\ & K \end{bmatrix} \begin{bmatrix} \widehat{V} \\ \widehat{U} \end{bmatrix} = \widehat{U}^{\mathrm{T}} K \widehat{U} + \widehat{V}^{\mathrm{T}} M \widehat{V},$$

where

$$\begin{bmatrix} \widehat{V} \\ \widehat{U} \end{bmatrix} = J^{\mathrm{T}} \begin{bmatrix} U \\ V \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} U + V \\ U - V \end{bmatrix}.$$

Therefore

$$\begin{aligned} &\inf_{\widehat{U}^{\mathrm{T}} E_+ \widehat{V} = I_k} \operatorname{trace}(\widehat{U}^{\mathrm{T}} K \widehat{U} + \widehat{V}^{\mathrm{T}} M \widehat{V}) \\ &= \inf_{(U-V)^{\mathrm{T}} E_+ (U+V) = 2I_k} \operatorname{trace}\left(\begin{bmatrix} U \\ V \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} A & B \\ B & A \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix}\right), \end{aligned} \tag{3.8}$$

where $E_\pm = \Sigma \pm \Delta$. We claim

$$(U - V)^{\mathrm{T}} E_+ (U + V) = 2I_k \quad \Leftrightarrow \quad (3.7). \tag{3.9}$$

This is because $(U - V)^{\mathrm{T}} E_+ (U + V) = 2I_k$ and its transpose version give

$$U^{\mathrm{T}} E_+ U + U^{\mathrm{T}} E_+ V - V^{\mathrm{T}} E_+ U - V^{\mathrm{T}} E_+ V = 2I_k, \tag{3.10a}$$

$$U^{\mathrm{T}} E_- U + V^{\mathrm{T}} E_- U - U^{\mathrm{T}} E_- V - V^{\mathrm{T}} E_- V = 2I_k. \tag{3.10b}$$

Add both equations in (3.10) and subtract one from the other to get

$$\begin{aligned} U^{\mathrm{T}}\Sigma U + U^{\mathrm{T}}\Delta V - V^{\mathrm{T}}\Delta U - V^{\mathrm{T}}\Sigma V &= 2I_k, \\ U^{\mathrm{T}}\Delta U - V^{\mathrm{T}}\Sigma U + U^{\mathrm{T}}\Sigma V - V^{\mathrm{T}}\Delta V &= 0. \end{aligned}$$

They are equivalent to (3.7). Equation (3.6) is now a consequence of Theorem 3.2, (3.8), and (3.9). □

3.2 Cauchy-like interlacing inequalities

The following theorem can be regarded as an extension of Cauchy's interlacing inequalities for the symmetric eigenvalue problem.

Theorem 3.4 *Let $U, V \in \mathbb{R}^{n\times k}$ such that $W \overset{def}{=} U^{\mathrm{T}}E_+V$ is nonsingular. Factorize $W = W_1^{\mathrm{T}}W_2$, where $W_i \in \mathbb{R}^{k\times k}$ are nonsingular, and define H_{SR} by (2.16). Denote by $\pm\mu_i$ for $1 \le i \le k$ the eigenvalues of H_{SR}, where $0 \le \mu_1 \le \cdots \le \mu_k$. Then*

$$\lambda_i \le \mu_i \le \beta\,\lambda_{i+n-k} \quad \text{for } 1 \le i \le k, \tag{3.11}$$

where $\beta = \sqrt{\min\{\kappa(\mathcal{K}), \kappa(\mathcal{M})\}}/\cos\angle(C^{\mathrm{T}}\mathcal{U}, D^{\mathrm{T}}\mathcal{V})$, $\kappa(X) \overset{def}{=} \|X\|_2\|X^{-1}\|_2$ is the spectral condition number of the matrix X, $\mathcal{U} = \mathrm{span}(U)$ and $\mathcal{V} = \mathrm{span}(V)$, and $\angle(C^{\mathrm{T}}\mathcal{U}, D^{\mathrm{T}}\mathcal{V})$ is the angle between $C^{\mathrm{T}}\mathcal{U}$ and $D^{\mathrm{T}}\mathcal{V}$.

Furthermore, if $\lambda_k < \lambda_{k+1}$ and $\lambda_i = \mu_i$ for $1 \le i \le k$, then

1. *$\mathcal{U} = \mathrm{span}(C^{-\mathrm{T}}\mathcal{X}_{(1:k,:)})$ when[3] $M \succ 0$, where $\mathcal{X}$ is as in Theorem 2.2;*
2. *$\{\mathcal{U}, \mathcal{V}\}$ is a pair of deflating subspaces of $H - \lambda E$ corresponding to the eigenvalues $\pm\lambda_i$ for $1 \le i \le k$ of (1.5) when both $K,\ M \succ 0$.*

Proof Apply [2, Theorem 4.1] to the eigenvalue problem for $\mathcal{H}$ in (2.2). □

The inequalities in (3.11) mirror Cauchy's interlacing inequalities for the symmetric eigenvalue problem. But the upper bound on μ_i by (3.11) is more complicated. The factor $[\cos\angle(C^{\mathrm{T}}\mathcal{U}, D^{\mathrm{T}}\mathcal{V})]^{-1}$ in general cannot be removed according to the example in [2, Remark 4.2] for the case $C = D = I$.

Theorem 3.5 *Under the assumptions of Theorem 3.4, if either $E_-\mathcal{U} \subseteq M\mathcal{V}$ when $M \succ 0$ or $E_+\mathcal{V} \subseteq K\mathcal{U}$ when $K \succ 0$, then*

$$\lambda_i \le \mu_i \le \lambda_{i+n-k} \quad \text{for } 1 \le i \le k. \tag{3.12}$$

Proof Note that

$$E_-\mathcal{U} \subseteq M\mathcal{V} \Leftrightarrow C^{\mathrm{T}}\mathcal{U} \subseteq \mathcal{M}D^{\mathrm{T}}\mathcal{V}, \quad E_+\mathcal{V} \subseteq K\mathcal{U} \Leftrightarrow D^{\mathrm{T}}\mathcal{V} \subseteq \mathcal{K}C^{\mathrm{T}}\mathcal{U}$$

and then apply [2, Theorem 4.3] to the eigenvalue problem for $\mathcal{H}$ in (2.2). □

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[3] A similar statement for the case in which $K \succ 0$ but $M \succeq 0$ can be made, noting that the decompositions in (2.7) no longer hold but similar decompositions exist.

4 Best approximations by a pair of subspaces

Recall the default assumption that $K,\ M \succeq 0$ and one of them is definite. Let $\{\mathcal{U}, \mathcal{V}\}$ be a pair of approximate deflating subspaces of $H - \lambda E$ and $\dim(\mathcal{U}) = \ell_1$ and $\dim(\mathcal{V}) = \ell_2$. Motivated by the minimization principles in Theorems 3.1 and 3.2, we would seek the best approximations to λ_j for $1 \le j \le k$ in the sense of

$$\frac{1}{2} \inf_{\substack{\widehat{U}^{\mathrm{T}} E_+ \widehat{V} = I_k \\ \operatorname{span}(\widehat{U}) \subseteq \mathcal{U}, \operatorname{span}(\widehat{V}) \subseteq \mathcal{V}}} \operatorname{trace}(\widehat{U}^{\mathrm{T}} K \widehat{U} + \widehat{V}^{\mathrm{T}} M \widehat{V}) \tag{4.1}$$

and their associated approximate eigenvectors. Necessarily $k \le \ell$. To this end, we divide our investigation into two cases. Let $U \in \mathbb{R}^{n \times \ell_1}$, $V \in \mathbb{R}^{n \times \ell_2}$ be the basis matrices of $\mathcal{U}$ and $\mathcal{V}$, respectively, and set $W = U^{\mathrm{T}} E_+ V$. The two cases are

1. W is nonsingular. Necessarily, $\ell_1 = \ell_2$. Set $\ell = \ell_1$.
2. W is singular or $\ell_1 \neq \ell_2$.

For the first case, i.e., W is nonsingular, let us factorize $W = W_1^{\mathrm{T}} W_2$, where $W_i \in \mathbb{R}^{\ell \times \ell}$ are nonsingular[4]. Note that any $\widehat{U}$ and $\widehat{V}$ such that $\operatorname{span}(\widehat{U}) \subseteq \mathcal{U}$, $\operatorname{span}(\widehat{V}) \subseteq \mathcal{V}$, and $\widehat{U}^{\mathrm{T}} E_+ \widehat{V} = I_k$ can be written as

$$\widehat{U} = U W_1^{-1} \widehat{X}, \quad \widehat{V} = V W_2^{-1} \widehat{Y},$$

where $\widehat{X}, \widehat{Y} \in \mathbb{R}^{\ell \times k}$ and $\widehat{X}^{\mathrm{T}} \widehat{Y} = I_k$, and vice versa. Hence we have

$$\widehat{U}^{\mathrm{T}} K \widehat{U} + \widehat{V}^{\mathrm{T}} M \widehat{V} = \widehat{X}^{\mathrm{T}} W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1} \widehat{X} + \widehat{Y}^{\mathrm{T}} W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1} \widehat{Y}$$

and thus

$$\begin{aligned} &\inf_{\substack{\widehat{U}^{\mathrm{T}} E_+ \widehat{V} = I_k \\ \operatorname{span}(\widehat{U}) \subseteq \mathcal{U}, \operatorname{span}(\widehat{V}) \subseteq \mathcal{V}}} \operatorname{trace}(\widehat{U}^{\mathrm{T}} K \widehat{U} + \widehat{V}^{\mathrm{T}} M \widehat{V}) \\ &\quad = \inf_{\widehat{X}^{\mathrm{T}} \widehat{Y} = I_k} \operatorname{trace}(\widehat{X}^{\mathrm{T}} W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1} \widehat{X} + \widehat{Y}^{\mathrm{T}} W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1} \widehat{Y}). \end{aligned} \tag{4.2}$$

By Theorem 3.2, we know that the right-hand side of (4.2) is the sum of the k smallest eigenvalues with the positive sign of H_{SR} defined earlier in subsection 2.2:

$$H_{\mathrm{SR}} = \begin{bmatrix} 0 & W_1^{-\mathrm{T}} U^{\mathrm{T}} K U W_1^{-1} \\ W_2^{-\mathrm{T}} V^{\mathrm{T}} M V W_2^{-1} & 0 \end{bmatrix} \in \mathbb{R}^{2\ell \times 2\ell}. \tag{2.16}$$

In summary, the *best approximations to the first k eigenvalues with the positive sign of $H - \lambda E$ within the pair of approximate deflating subspaces are those of* H_{SR}.

[4] How this factorization is done is not essential mathematically. But it is included to accommodate cases when such a factorization may offer certain conveniences. In general, simply taking $W_1 = W^{\mathrm{T}}$ and $W_2 = I_\ell$ or $W_1 = I_\ell$ and $W_2 = W$ may be sufficient.

Algorithmically, denote by μ_j ($j = 1, \ldots, \ell$) the eigenvalues with the positive sign of $H_{\rm SR}$ in the ascending order, i.e., $0 \le \mu_1 \le \cdots \le \mu_\ell$, and by $\hat{z}_j$ the associated eigenvectors:

$$H_{\rm SR}\hat{z}_j = \mu_j\hat{z}_j, \quad \hat{z}_j = \begin{bmatrix} \hat{y}_j \\ \hat{x}_j \end{bmatrix}. \tag{4.3}$$

It can be verified that

$$\rho(UW_1^{-1}\hat{x}_j, VW_2^{-1}\hat{y}_j) = \mu_j \quad \text{for } j = 1, \ldots, \ell.$$

Naturally, according to Algorithm 2.1, we take $\lambda_j \approx \mu_j$ and the corresponding approximate eigenvectors of $H - \lambda E$ as

$$\tilde{z}_j \equiv \begin{bmatrix} \tilde{y}_j \\ \tilde{x}_j \end{bmatrix} = \begin{bmatrix} VW_2^{-1}\hat{y}_j \\ UW_1^{-1}\hat{x}_j \end{bmatrix} \quad \text{for } j = 1, \ldots, \ell. \tag{4.4}$$

In practice, not all of the approximate eigenpairs $(\mu_j, \tilde{z}_j)$ are equally accurate to the same level. Usually the first few pairs are more accurate than the next few.

For the ease of reference, we summarize the above findings into the following theorem.

Theorem 4.1 *Let $\{\mathcal{U}, \mathcal{V}\}$ be a pair of approximate deflating subspaces of $H - \lambda E$ with $\dim(\mathcal{U}) = \dim(\mathcal{V}) = \ell$, and let $U,\ V \in \mathbb{R}^{n\times\ell}$ be the basis matrices of $\mathcal{U}$ and $\mathcal{V}$, respectively. If $W \overset{def}{=} U^{\rm T}E_+V$ is nonsingular, then the best approximations to λ_j for $1 \le j \le k$ in the sense of (4.1) are the eigenvalues μ_j of H_{SR} defined in (2.16) with the corresponding approximate eigenvectors given by (4.4), and*

$$\sum_{j=1}^{k}\mu_j = \frac{1}{2} \inf_{\substack{\widehat{U}^{\rm T}E_+\widehat{V}=I_k \\ \text{span}(\widehat{U})\subseteq\mathcal{U}, \text{span}(\widehat{V})\subseteq\mathcal{V}}} \text{trace}(\widehat{U}^{\rm T}K\widehat{U} + \widehat{V}^{\rm T}M\widehat{V}).$$

The next theorem turns the eigenvalue problem of $H_{\rm SR}$ into a generalized eigenvalue problem of the same kind as $H - \lambda E$. We omit its proof because of its simplicity.

Theorem 4.2 *Let $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times k}$ such that $W \overset{def}{=} U^{\rm T}E_+V$ is nonsingular, and define H_{SR} as in (2.16). Then the eigenvalues of H_{SR} are same as those of the matrix pencil*

$$\begin{bmatrix} U & \\ & V \end{bmatrix}^{\rm T} (H - \lambda E) \begin{bmatrix} V & \\ & U \end{bmatrix} = \begin{bmatrix} & U^{\rm T}KU \\ V^{\rm T}MV & \end{bmatrix} - \lambda \begin{bmatrix} U^{\rm T}E_+V & \\ & V^{\rm T}E_-U \end{bmatrix}, \tag{4.5}$$

and the eigenvectors $\hat{z}$ of H_{SR} and those $\check{z}$ of the pencil are related by $\hat{z} = (W_2 \oplus W_1)\check{z}$.

Remark 4.1 The best approximation technique so far is based on the minimization principles in Theorems 3.1 and 3.2. Naturally one may wonder if a similar technique could be devised using the minimization principles in Theorem 3.3 for the original LR eigenvalue problem (1.4). But that seems hard if we seek to project each individual matrices A, B, Δ, and Σ separately. Alternatively, we may resort to Theorem 4.2 by recasting the projection in (4.5) back to the original LR eigenvalue problem (1.4). The resulting scheme turns out to be the projection idea in [14], where Olsen, Jensen, and Jørgensen [14] were simply aiming at producing a much smaller projected problem of the same kind in the form of (1.4). Note that Theorem 3.3 was not yet known in 1988 and thus it was not possible in [14] to investigate any issue regarding the best possible approximations in the sense of the theorem. What we are doing here is to not only produce a much smaller projected problem of the same kind in form as (1.5) but also make sure the projected problem to give the best possible approximations to the desired eigenvalues. Despite that we seek our projection scheme to achieve multiple goals, the end result is not essentially different from the one in [14]. That is remarkable. ◊

It turns out the second case (namely W is singular or $\ell_1 \neq \ell_2$) is much more complicated, but the conclusion is similar in that the optimization problem (4.1) can still be solved through solving a smaller eigenvalue problem for a projection matrix $\widehat{H}_{\rm SR}$ to be defined in Appendix A, where Theorem 8.1 similar to Theorem 4.1 will be presented.

5 Locally optimal 4-D CG algorithms

5.1 4-D search

Line search is a common approach in the process of optimizing a function value. For our case, we are interested in solving

$$\inf_{x,y} \rho(x, y) = \inf_{x,y} \frac{x^{\rm T} K x + y^{\rm T} M y}{2|x^{\rm T} E_+ y|} \tag{5.1}$$

in order to compute λ_1 and its associated eigenvector of $H - \lambda E$.

Given a search direction $\begin{bmatrix} q \\ p \end{bmatrix}$ from the current position $\begin{bmatrix} y \\ x \end{bmatrix}$, the basic idea of the standard line search is to look for the best possible scalar argument t on the line

$$\left\{ \begin{bmatrix} y \\ x \end{bmatrix} + t \begin{bmatrix} q \\ p \end{bmatrix} \;:\; t \in \mathbb{R} \right\} \tag{5.2}$$

to minimize ρ:

$$\min_t \rho(x + tp, y + tq). \tag{5.3}$$

For the steepest descent method, the search directions p and q are the gradients [1] of $\rho(x, y)$ with respect to x and y:

$$\nabla_x \rho = \frac{1}{x^{\mathrm{T}} E_+ y} \left[Kx - \rho(x, y)\, E_+ y \right], \; \nabla_y \rho = \frac{1}{x^{\mathrm{T}} E_+ y} \left[My - \rho(x, y)\, E_- x \right]. \tag{5.4}$$

Note that there is a close relation between these two gradients and the residual:

$$Hz - \rho(x, y) Ez = x^{\mathrm{T}} E_+ y \begin{bmatrix} \nabla_x \rho \\ \nabla_y \rho \end{bmatrix}. \tag{5.5}$$

Namely the block vector obtained by stacking $\nabla_x \rho$ over $\nabla_y \rho$ is parallel to the residual.

The idea of the dual-channel line search in [4] for the case $E = I_{2n}$ can be readily extended to solve the minimization problem

$$\min_{s,t} \rho(x + sp, y + tq). \tag{5.6}$$

It goes as follows: solve (5.6) iteratively by freezing one of s and t and minimize the functional ρ over the other in an alternative manner. Choices of p and q in (5.6) include the gradients $\nabla_x \rho$ and $\nabla_y \rho$ as well.

However we did not pursue these ideas for the reasons as discussed in [3]. Instead, we look for four scalars α, β, s, and t to minimize $\rho(\alpha x + sp, \beta y + tq)$. This no longer performs a line or dual search, but a *4-dimensional subspace search*:

$$\inf_{\alpha,\beta,s,t} \rho(\alpha x + sp, \beta y + tq) = \min_{u \in \mathrm{span}(U),\; v \in \mathrm{span}(V)} \rho(u, v), \tag{5.7}$$

within the *4-dimensional subspace*

$$\left\{ \begin{bmatrix} \beta y + tq \\ \alpha x + sp \end{bmatrix} \quad \text{for all scalars } \alpha, \beta, s, \text{and } t \right\}, \tag{5.8}$$

where $U = [x, p] \in \mathbb{R}^{n \times 2}$ and $V = [y, q] \in \mathbb{R}^{n \times 2}$. The right-hand side of (5.7) can be solved by the methods given in section 4 if $U^{\mathrm{T}} E_+ V$ is nonsingular (the common case) or in Appendix A otherwise.

5.2 Algorithms

The minimization principle (3.3)/(3.4), and the one in Theorem 3.2 make it tempting to apply steepest descent (SD) or nonlinear CG algorithms [13] to solve the LR eigenvalue problem. For the case $\Sigma = I_n$ and $\Delta = 0$ (which corresponds to $E = I_{2n}$), such applications had been attempted in [10,12] to solve the LR eigenvalue problem (1.2). Conceivably when only one eigenvalue and its associated eigenvector are requested, it matters little, if any, to apply CG to $\rho(x, y)$ based on (3.3) for the eigenvalue problem (1.5) or to $\varrho(u, v)$ based on (3.4) for the original eigenvalue problem (1.4). But it is a very different story if more than one eigenpair are requested, in which case block algorithms are better options. As in [3] which is for the case $E = I_{2n}$, we will present *locally optimal 4-D CG algorithms* for the current case, based on the minimization principle (3.5) and the Cauchy-like interlacing inequalities in Theorem 3.4. This is Algorithm 5.1 below, collectively called the *Locally Optimal Block Preconditioned 4-D CG Algorithm* (LOBP4DCG), where $k = 1$ or $k > 1$ corresponds to a no-block or block version, and

$$\Phi = \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix} \tag{5.9}$$

or some nontrivial ones corresponds to a no-preconditioned or preconditioned version.

Algorithm 5.1 The *locally optimal 4-D CG algorithms:*

0 Given initial approximations X_0 and Y_0 having k columns such that columns of $Z_0 = \begin{bmatrix} Y_0 \\ X_0 \end{bmatrix}$ are approximate eigenvectors of $H - \lambda E$ associated with λ_j, $1 \le j \le k$.
1 for $i = 0, 1, \dots$ until convergence:
2 $\rho_j = \rho((X_i)_{(:,j)}, (Y_i)_{(:,j)})$, $1 \le j \le k$;
3 $P_i = K X_i - E_+ Y_i \ \mathrm{diag}(\rho_1, \dots, \rho_k)$,
$Q_i = M Y_i - E_- X_i \ \mathrm{diag}(\rho_1, \dots, \rho_k)$;
3.1 $\begin{bmatrix} Q_i \\ P_i \end{bmatrix} \leftarrow \Phi \begin{bmatrix} P_i \\ Q_i \end{bmatrix}$ if the preconditioner Φ is given;
4.1 For $i = 0$: $U = [X_i, P_i]$, $V = [Y_i, Q_i]$;
4.2 For $i > 0$: $U = [X_i, X_{i-1}, P_i]$, $V = [Y_i, Y_{i-1}, Q_i]$;
4.3 Orthogonalize the columns of U and V;
4.4 $W = U^{\mathrm{T}} E_+ V = W_1^{\mathrm{T}} W_2$;
5 Construct H_{SR} as in (2.16) (assume W is nonsingular);
6 Compute the k smallest eigenvalues with the positive sign of H_{SR}, and the associated eigenvectors as in (4.3);
7 $X_{i+1} = U W_1^{-1} [\hat{x}_1, \dots, \hat{x}_k]$, $Y_{i+1} = V W_2^{-1} [\hat{y}_1, \dots, \hat{y}_k]$;
8 Normalize each column of $Z_{i+1} = \begin{bmatrix} Y_{i+1} \\ X_{i+1} \end{bmatrix}$.
9 end

Most comments we made for [3, Algorithm 4.1] there apply here (see also [1]). But we will briefly discuss the choosing of a preconditioner Φ. Taking Φ as in (5.9) means no preconditioner. In general, a *generic* preconditioner to compute the eigenvalues of $H - \lambda E$ near a prescribed point μ is

$$\Phi = (H - \mu E)^{-1}.$$

When μ is closer to the desired eigenvalues than any others, the preconditioned directions should have "larger" components in the desired eigenvectors than the ones obtained without preconditioning. Since we are particularly interested in the smallest eigenvalues with the positive sign, $\mu = 0$ is often an obvious choice. Then

$$\Phi \begin{bmatrix} \nabla_x \rho \\ \nabla_y \rho \end{bmatrix} = \begin{bmatrix} 0 & M^{-1} \\ K^{-1} & 0 \end{bmatrix} \begin{bmatrix} \nabla_x \rho \\ \nabla_y \rho \end{bmatrix} = \begin{bmatrix} M^{-1} \nabla_y \rho \\ K^{-1} \nabla_x \rho \end{bmatrix} \equiv \begin{bmatrix} q \\ p \end{bmatrix}. \tag{5.10}$$

In this case, both p and q can be computed by using the conjugate gradient method [6,8].

6 Numerical results

In this section, we present some numerical results to illustrate the essential convergence behaviors of locally optimal 4-D CG algorithms in Sect. 5. The matrices $K, M \succ 0$ in the LR problem (1.5) are chosen from [5], and E_+ is a sparse random matrix E_+. Specifically, $n = 3,600$, K is `bcsstk21`, and M is the $n \times n$ leading principle matrix of `sts4098`, $E_+ =$ `sprandn(n, n, 0.1)` in MATLAB. Both K and M are first symmetrically permuted through MATLAB's `symamd` (symmetric approximate minimum degree permutation) in attempt to reduce the numbers of fill-ins in their respective incomplete Cholesky decompositions.

Our goal is to compute 4 smallest positive eigenvalues $0 < \lambda_1 < \lambda_2 < \lambda_3 < \lambda_4$ and corresponding eigenvectors z_1, z_2, z_3, z_4 of $H - \lambda E$. The initial approximate eigenvectors of z_i are randomly chosen. Two different preconditioners are used to approximate

$$H^{-1} = \begin{bmatrix} 0 & M^{-1} \\ K^{-1} & 0 \end{bmatrix}.$$

The first preconditioner Φ_1 is constructed through incomplete Cholesky decompositions of K and M:

$$\Phi_1 = \begin{bmatrix} 0 & (R_M^{\mathrm{T}} R_M)^{-1} \\ (R_K^{\mathrm{T}} R_K)^{-1} & 0 \end{bmatrix},$$

where R_K and R_M are the incomplete Cholesky decomposition factors, respectively. It turns out that both `cholinc(K,'0')` and `cholinc(M,'0')` with no fill-ins do not exists; so we end up using

$$R_K = \texttt{cholinc(K, tol)}, \quad R_M = \texttt{cholinc(K, tol)} \tag{6.1}$$

with a tolerance `tol`. Among various `tol` we tested, we found that for `tol` $= 10^{-4}$ or smaller, Φ_1 works very well, but not so for `tol` $= 10^{-3}$ or bigger. In the reported results below, `tol` $= 10^{-4}$.

The second preconditioner Φ_2 is via applying H^{-1} approximately by calculating the preconditioned vectors p and q as in (5.10) by the preconditioned linear CG method [6,8] with stopping tolerance 10^{-2} on the associated normalized residual norms or maximum 20 iterations. The preconditioners for calculating p and q are $(R_K^{\mathrm{T}} R_K)^{-1}$ and $(R_M^{\mathrm{T}} R_M)^{-1}$, respectively, with again R_K and R_M as given by (6.1). Note both K and M are very ill-conditioned: $\kappa(K) = 4.5 \cdot 10^7$ and $\kappa(M) = 4.3 \cdot 10^8$.

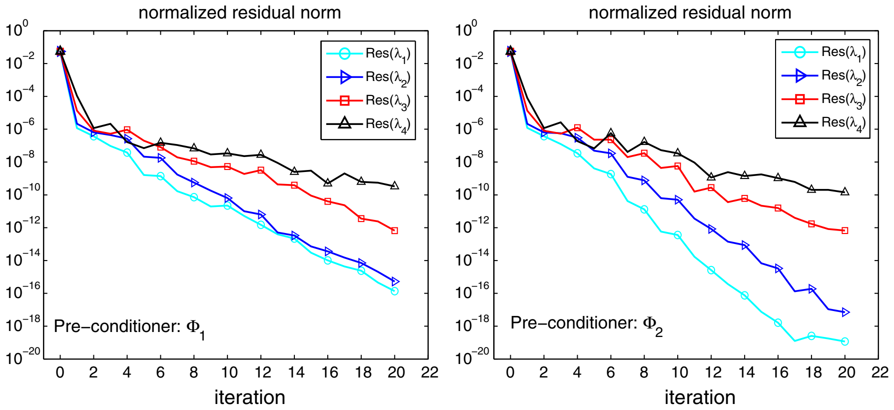

Fig. 1 The convergence behaviors of the locally optimal block 4-D preconditioned CG algorithms for computing the 4 smallest positive eigenvalues of an made-up LR problem.

The plain (i.e., without a suitable preconditioner) linear CG iteration for computing p and q converges extremely slowly. But the preconditioners $(R_K^{\mathrm{T}}R_K)^{-1}$ and $(R_M^{\mathrm{T}}R_M)^{-1}$ with modest fill-in tolerance 10^{-3} are sufficient for the linear CG iteration.

Note that Φ_1 can be regarded as a Φ_2 with using just one step of the linear CG to compute the preconditioned vectors p and q. This explains why a smaller `tol` in (6.1) is needed for constructing Φ_1, while a larger `tol` in (6.1) for constructing Φ_2 is fine so long as the associated linear systems are solved with adequate accuracy (recall the stopping tolerance 10^{-2}).

Figure 1 shows the normalized residual norms of a MATLAB implementation of Algorithm 5.1 with the preconditioners Φ_1 and Φ_2. The normalized residual norms for the jth approximate eigenpair $(\lambda_j^{(i)}, z_j^{(i)})$ at the ith iterative step are defined by

$$\frac{\|Hz_j^{(i)} - \lambda_j^{(i)}Ez_j^{(i)}\|_1}{(\|H\|_1 + \lambda_j^{(i)}\|E\|_1)\|z_j^{(i)}\|_1},$$

where $\|\cdot\|_1$ is the ℓ_1-norm of a vector or the ℓ_1-operator norm of a matrix. We observe rather steady convergence towards the desired 4 eigenpairs. Other examples we have run but not reported here show similar behavior.

7 Concluding remarks

We have presented minimization principles and Cauchy-like interlacing inequalities for the generalized LR eigenvalue problem. These new results mirror the three well-known results for the eigenvalue problem of a real symmetric matrix, and enable us to devise new efficient numerical methods for computing the first few smallest eigenvalues with the positive sign and corresponding eigenvectors simultaneously.

Although, throughout this paper, it is assumed K, M, and $E_\pm$ are real matrices, all results are valid for Hermitian positive semi-definite K and M with one of them being definite after minor changes: replacing all $\mathbb{R}$ by $\mathbb{C}$ and all superscripts $(\cdot)^{\mathrm{T}}$ by complex conjugate transposes $(\cdot)^{\mathrm{H}}$.

The numerical results in Sect. 6 demonstrates the effectiveness of the new algorithms. Although they are for an artificial generalized LR problem. we argue that its numerical behavior is rather suggestive. In the future, we would like to test the proposed method on realistic LR eigenvalue problems arising from the excited states calucation in computational quantum physics [14].

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Appendix: Best approximations: the singular/unequal dimension case

This appendix continues the investigation in Sect. 4 to seek best approximate eigenpairs of $H - \lambda E$ for given $\{\mathcal{U}, \mathcal{V}\}$, a pair of approximate deflating subspaces of $H - \lambda E$ with $\dim(\mathcal{U}) = \ell_1$ and $\dim(\mathcal{V}) = \ell_2$. In Sect. 4, we have treated the case in which $\ell_1 = \ell_2$ and $W \stackrel{\text{def}}{=} U^{\mathrm{T}} E_+ V$ is nonsingular, where $U \in \mathbb{R}^{n\times\ell_1}$, $V \in \mathbb{R}^{n\times\ell_2}$ are the basis matrices of $\mathcal{U}$ and $\mathcal{V}$, respectively. In what follows, we will focus on the general case: ℓ_1 and ℓ_2 are not necessarily equal or W may be singular.

The case is much more complicated than the one in section 4, but it can be handled in the similar way as in [3] which is for $E = I_{2n}$. So we will simply summarize the results and the reader is referred to [1, Appendix A] for detail.

Factorize

$$W = W_1^{\mathrm{T}} W_2, \quad W_i \in \mathbb{R}^{r\times\ell_i}, \quad r = \operatorname{rank}(W) \le \min_i \ell_i. \tag{8.1}$$

Both W_i have full row rank. Factorize[5]

$$W_i^{\mathrm{T}} = Q_i \begin{bmatrix} R_i \\ 0 \end{bmatrix} \quad \text{for} i = 1, 2, \tag{8.2}$$

where $R_i \in \mathbb{R}^{r\times r}$, $Q_i \in \mathbb{R}^{\ell_i\times\ell_i}$ $(i = 1, 2)$ are nonsingular. Partition

$$Q_1^{-1} U^{\mathrm{T}} K U Q_1^{-\mathrm{T}} = \begin{array}{c} \\ r \\ \ell_1-r \end{array} \!\!\begin{array}{c} \begin{array}{cc} r & \ell_1-r \end{array} \\ \begin{bmatrix} K_{11} & K_{12} \\ K_{12}^{\mathrm{T}} & K_{22} \end{bmatrix} \end{array}, \tag{8.3a}$$

$$Q_2^{-1} V^{\mathrm{T}} M V Q_2^{-\mathrm{T}} = \begin{array}{c} \\ r \\ \ell_2-r \end{array} \!\!\begin{array}{c} \begin{array}{cc} r & \ell_2-r \end{array} \\ \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^{\mathrm{T}} & M_{22} \end{bmatrix} \end{array}. \tag{8.3b}$$

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[5] Computationally, this can be realized by the QR decompositions of W_i^{T}. For more generality in presentation, we do not assume that they have to be QR decompositions.

Set

$$\widehat{H}_{\rm SR} = \begin{bmatrix} 0 & R_1^{-1}\mathcal{K}_{11}R_1^{-\rm T} \\ R_2^{-1}\mathcal{M}_{11}R_2^{-\rm T} & 0 \end{bmatrix} \in \mathbb{R}^{2r\times 2r}, \tag{8.4}$$

where $K_{22}^{\dagger}$ and $M_{22}^{\dagger}$ are the Moore-Penrose inverses of K_{22} and M_{22}, respectively, and

$$\mathcal{K}_{11} = K_{11} - K_{12}K_{22}^{\dagger}K_{12}^{\rm H}, \quad \mathcal{M}_{11} = M_{11} - M_{12}M_{22}^{\dagger}M_{12}^{\rm H}. \tag{8.5}$$

Denote by μ_j for $j = 1, \dots, r$ the eigenvalues with the positive sign of $\widehat{H}_{\rm SR}$ in the ascending order and by $\hat{z}_j$ the associated eigenvectors:

$$\widehat{H}_{\rm SR}\hat{z}_j = \mu_j\hat{z}_j, \quad \hat{z}_j = \begin{bmatrix} \hat{y}_j \\ \hat{x}_j \end{bmatrix}. \tag{8.6}$$

It can be verified that $\rho(\tilde{x}_j, \tilde{y}_j) = \mu_j \quad \text{for} j = 1, \dots, r$, where

$$\tilde{x}_j = UQ_1^{-\rm T}\begin{bmatrix} R_1^{-\rm T}\hat{x}_j \\ u_j \end{bmatrix}, \quad \tilde{y}_j = VQ_2^{-\rm T}\begin{bmatrix} R_2^{-\rm T}\hat{y}_j \\ v_j \end{bmatrix} \tag{8.7}$$

for any u_j and v_j satisfying

$$K_{22}u_j = -K_{12}^{\rm T}R_1^{-\rm T}\hat{x}_j, \quad M_{22}v_j = -M_{12}^{\rm T}R_2^{-\rm T}\hat{y}_j. \tag{8.8}$$

Naturally the approximate eigenvectors of $H - \lambda E$ should be taken as

$$\tilde{z}_j = \begin{bmatrix} \tilde{y}_j \\ \tilde{x}_j \end{bmatrix} \quad \text{for} j = 1, \dots, r. \tag{8.9}$$

Theorem 8.1 *Let* $\{\mathcal{U}, \mathcal{V}\}$ *be a pair of approximate deflating subspaces of* $H - \lambda E$ *with* $\dim(\mathcal{U}) = \ell_1$ *and* $\dim(\mathcal{V}) = \ell_2$, *and let* $U \in \mathbb{R}^{n\times \ell_1}$, $V \in \mathbb{R}^{n\times \ell_2}$ *be the basis matrices of* $\mathcal{U}$ *and* $\mathcal{V}$, *respectively. Let* $\widehat{H}_{SR}$ *be defined by* (8.4). *Then the best approximations to* λ_j *for* $1 \le j \le k$ *in the sense of* (4.1) *are the corresponding eigenvalues of* $\widehat{H}_{SR}$, *with the corresponding approximate eigenvectors given by* (8.7)–(8.9).

Despite much more complicated appearance of $\widehat{H}_{\rm SR}$ compared to $H_{\rm SR}$ in Sect. 4, our next theorem surprisingly unifies both.

Theorem 8.2 *The eigenvalues of* $\widehat{H}_{SR}$ *in* (8.4) *are the same as the finite eigenvalues of*

$$\begin{aligned} \check{H} - \lambda\check{E} := &\begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix}^{\rm T}(H - \lambda E)\begin{bmatrix} V & 0 \\ 0 & U \end{bmatrix} \\ = &\begin{bmatrix} 0 & U^{\rm T}KU \\ V^{\rm T}MV & 0 \end{bmatrix} - \lambda\begin{bmatrix} U^{\rm T}E_+V & \\ & V^{\rm T}E_-U \end{bmatrix} \end{aligned} \tag{8.10}$$

and the eigenvector $\hat{z} = \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix}$ *of* $\widehat{H}_{SR}$ *and the eigenvector* $\check{z} = \begin{bmatrix} \check{y} \\ \check{x} \end{bmatrix}$ *of the pencil* (8.10) *associated with a finite eigenvalue are related by*

$$\check{x} = Q_1^{-\mathrm{T}} \begin{bmatrix} R_1^{-\mathrm{T}} \hat{x} \\ -K_{22}^{\dagger} K_{12}^{\mathrm{T}} R_1^{-\mathrm{T}} \hat{x} + g \end{bmatrix}, \quad \check{y} = Q_2^{-\mathrm{T}} \begin{bmatrix} R_2^{-\mathrm{T}} \hat{y} \\ -M_{22}^{\dagger} M_{12}^{\mathrm{T}} R_2^{-\mathrm{T}} \hat{y} + h \end{bmatrix}, \tag{8.11}$$

where g *is any vector in the kernel of* K_{22} *and* h *is any vector in the kernel of* M_{22}*. In particluar, if* $\ell_1 = \ell_2 = r$*, the relation in* (8.11) *is simplified to* $\hat{z} = (W_2 \oplus W_1)\check{z}$ *as in Theorem 4.2.*

Proof Let $P_i = Q_i^{-\mathrm{T}}(R_i^{-\mathrm{T}} \oplus I_{\ell_i - r})$ for $i = 1, 2$ and both are nonsingular. It can be verified that

$$(P_1 \oplus P_2)^{\mathrm{T}} (\check{H} - \lambda \check{E})(P_2 \oplus P_1) = \begin{bmatrix} 0 & \widehat{K} \\ \widehat{M} & 0 \end{bmatrix} - \lambda \begin{bmatrix} \widehat{I} & \\ 0 & \widehat{I}^{\mathrm{T}} \end{bmatrix},$$

where

$$\widehat{M} = \begin{bmatrix} R_2^{-1} & \\ & I_{\ell_2 - r} \end{bmatrix} \begin{bmatrix} M_{11} & M_{12} \\ M_{12}^{\mathrm{T}} & M_{22} \end{bmatrix} \begin{bmatrix} R_2^{-\mathrm{T}} & \\ & I_{\ell_2 - r} \end{bmatrix}, \tag{8.12}$$

$$\widehat{K} = \begin{bmatrix} R_1^{-1} & \\ & I_{\ell_1 - r} \end{bmatrix} \begin{bmatrix} K_{11} & K_{12} \\ K_{12}^{\mathrm{T}} & K_{22} \end{bmatrix} \begin{bmatrix} R_1^{-\mathrm{T}} & \\ & I_{\ell_1 - r} \end{bmatrix}, \tag{8.13}$$

$$\widehat{I} = \begin{bmatrix} I_r \\ & 0 \end{bmatrix} \in \mathbb{R}^{\ell_1 \times \ell_2}, \tag{8.14}$$

and K_{ij} and M_{ij} are defined by 8.3. Since K and M are positive (semi)definite, we have $\operatorname{span}(K_{12}^{\mathrm{T}}) \subseteq \operatorname{span}(K_{22})$ and $\operatorname{span}(M_{12}^{\mathrm{T}}) \subseteq \operatorname{span}(M_{22})$ and consequently

$$K_{22} K_{22}^{\dagger} K_{12}^{\mathrm{T}} = K_{12}^{\mathrm{T}}, \quad M_{22} M_{22}^{\dagger} M_{12}^{\mathrm{T}} = M_{12}^{\mathrm{T}}. \tag{8.15}$$

Let

$$Z_1 = \begin{bmatrix} I_r & 0 \\ -K_{22}^{\dagger} K_{12}^{\mathrm{T}} R_1^{-\mathrm{T}} & I_{\ell_1 - r} \end{bmatrix}, \quad Z_2 = \begin{bmatrix} I_r & 0 \\ -M_{22}^{\dagger} M_{12}^{\mathrm{T}} R_2^{-\mathrm{T}} & I_{\ell_2 - r} \end{bmatrix}.$$

It can be verified that $Z_1^{\mathrm{T}} \widehat{I} Z_2 = \widehat{I}$ and, after using (8.15),

$$Z_1^{\mathrm{T}} \widehat{K} Z_1 = \begin{bmatrix} R_1^{-1} \mathcal{K}_{11} R_1^{-\mathrm{T}} & 0 \\ 0 & K_{22} \end{bmatrix}, \quad Z_2^{\mathrm{T}} \widehat{M} Z_2 = \begin{bmatrix} R_2^{-1} \mathcal{M}_{11} R_2^{-\mathrm{T}} & 0 \\ 0 & M_{22} \end{bmatrix},$$

where $\mathcal{K}_{11}$ and $\mathcal{M}_{11}$ are defined in (8.5). Hence $(P_1 Z_1 \oplus P_2 Z_2)^{\mathrm{T}}(\check{H} - \lambda \check{E})(P_2 Z_2 \oplus P_1 Z_1)$ is

$$\begin{array}{c} \\ r \\ \ell_1-r \\ r \\ \ell_2-r \end{array}\begin{array}{c} \begin{array}{cccc} r & \ell_2-r & r & \ell_1-r \end{array} \\ \begin{bmatrix} 0 & 0 & R_1^{-1}\mathcal{K}_{11}R_1^{-\mathrm{T}} & 0 \\ 0 & 0 & 0 & K_{22} \\ R_2^{-1}\mathcal{M}_{11}R_2^{-\mathrm{T}} & 0 & 0 & 0 \\ 0 & M_{22} & 0 & 0 \end{bmatrix} \end{array} - \lambda \begin{array}{c} \\ r \\ \ell_1-r \\ r \\ \ell_2-r \end{array}\begin{array}{c} \begin{array}{cccc} r & \ell_2-r & r & \ell_1-r \end{array} \\ \begin{bmatrix} I_r & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & I_r & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array} \tag{8.16}$$

whose finite eigenvalues are the eigenvalues of

$$\begin{bmatrix} 0 & R_1^{-1}\mathcal{K}_{11}R_1^{-\mathrm{T}} \\ R_2^{-1}\mathcal{M}_{11}R_2^{-\mathrm{T}} & 0 \end{bmatrix} - \lambda I_{2r} = \widehat{H}_{\mathrm{SR}} - \lambda I_{2r}. \tag{8.17}$$

Now we turn to look for the eigenvector relation. Given an eigenvector $\hat{z} = \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix}$ of $\widehat{H}_{\mathrm{SR}}$, we conclude by comparing (8.16) and (8.17) that the corresponding eigenvector of the matrix pencil (8.16) is

$$\begin{bmatrix} \hat{y} \\ h \\ \hat{x} \\ g \end{bmatrix},$$

where g is any vector in the kernel of K_{22} and h is any vector in the kernel of M_{22}. Therefore the corresponding eigenvector $\check{z} = \begin{bmatrix} \check{y} \\ \check{x} \end{bmatrix}$ of $\check{H} - \lambda \check{E}$ is given by

$$\check{x} = P_1 Z_1 \begin{bmatrix} \hat{x} \\ g \end{bmatrix}, \quad \check{y} = P_2 Z_2 \begin{bmatrix} \hat{y} \\ h \end{bmatrix}$$

which, after simplification, yields (8.11). □

The next theorem says that there are Cauchy-like interlacing inequalities for $\widehat{H}_{\mathrm{SR}}$, too. We omit its proof because its similarity to [3, Theorem 8.3] (see also [1, Appendix A]).

Theorem 8.3 *Assume the conditions of Theorem 8.1. Then*

$$\lambda_i \le \mu_i \le \lambda_{i+2n-(\ell_1+\ell_2)} \quad \mathit{for} 1 \le i \le r, \tag{8.18}$$

where $\lambda_{i+2n-(\ell_1+\ell_2)} = \infty$ *if* $i + 2n - (\ell_1 + \ell_2) > n$.

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