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Error bounds for approximate deflating subspaces for linear response eigenvalue problems

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ABSTRACT

Consider the linear response eigenvalue problem (LREP) for $H = \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix}$, where K and M are positive semidefinite and one of them is definite. Given a pair of approximate deflating subspaces of $\{K, M\}$, it can be shown that LREP can be transformed into one for $\widetilde{H}$ that is nearly decoupled into two smaller LREPs upon congruence transformations on K and M that preserve the eigenvalues of H. In this paper, we establish a bound on how far the pair of approximate deflating subspaces is from a pair of exact ones, using the closeness of $\widetilde{H}$ from being decoupled.

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Perturbation
Deflating subspaces

1. Introduction

In computational quantum chemistry and physics, the so-called *random phase approximation* (RPA) describes the excitation states (energies) of physical systems in the study of collective motion of many-particle systems [1–3]. It has important applications in silicon nanoparticles and nanoscale materials and analysis of interstellar clouds [1,4]. One important question in RPA is to compute a few eigenpairs associated with the smallest *positive* eigenvalues of the following eigenvalue problem:

$$\mathscr{H}\boldsymbol{w} := \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix}, \tag{1.1}$$

where $A, B \in \mathbb{R}^{n\times n}$ are both symmetric matrices and $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ is positive definite. Through a similarity transformation, this eigenvalue problem can be equivalently transformed into [1,4,5]

$$H\boldsymbol{z} := \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix}, \tag{1.2}$$

where $K = A - B$ and $M = A + B$. This eigenvalue problem was still referred to as the *linear response eigenvalue problem* (LREP) [1,5,6] and will be in this paper, too.

The condition imposed upon A and B in (1.1) implies that both K and M are symmetric and positive definite [1]. But in the rest of this paper, unless otherwise explicitly stated, we relax the positive definiteness of both K and M to that *both are positive semidefinite and one of them is definite.*

An important notion for LREP [1] is the so-called *pair of deflating subspaces* $\{\mathcal{U}, \mathcal{V}\}$ by which we mean that both $\mathcal{U}$ and $\mathcal{V}$ are subspaces of $\mathbb{R}^n$ and satisfy

$$K\mathcal{U} \subseteq \mathcal{V} \quad \text{and} \quad M\mathcal{V} \subseteq \mathcal{U}.$$

More discussions on this are in section 3. It is a generalization of the concept of the invariant subspace (or, eigenspace) in the standard eigenvalue problem upon considering the special structure in the LREP (1.2). This notion is not only vital in analyzing the theoretical properties such as the subspace version [1] of Thouless's minimization principle [2] and the Cauchy-like interlacing inequalities [4], but also fundamental for several rather efficient algorithms, e.g., the Locally Optimal Block Preconditioned 4D Conjugate Gradient Method (LOBP4DCG) [4] and its space-extended variation [7], the block Chebyshev–Davidson method [8], as well as the generalized Lanczos method [9, 10,6]. Each of these algorithms generates a sequence of approximate deflating subspace