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A symmetric structure-preserving ΓQR algorithm for linear response eigenvalue problems

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ABSTRACT

In this paper, we present an efficient ΓQR algorithm for solving the linear response eigenvalue problem $\mathscr{H}\boldsymbol{x} = \lambda\boldsymbol{x}$, where $\mathscr{H}$ is $\boldsymbol{\Pi}^{-}$-symmetric with respect to $\Gamma_0 = \mathrm{diag}(I_n, -I_n)$. Based on newly introduced Γ-orthogonal transformations, the ΓQR algorithm preserves the $\boldsymbol{\Pi}^{-}$-symmetric structure of $\mathscr{H}$ throughout the whole process, and thus guarantees the computed eigenvalues to appear pairwise $(\lambda, -\lambda)$ as they should. With the help of a newly established implicit Γ-orthogonality theorem, we incorporate the implicit multi-shift technique to accelerate the convergence of the ΓQR algorithm. Numerical experiments are given to show the effectiveness of the algorithm.

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1. Introduction

In this paper, we consider the standard eigenvalue problem of the form

$$\mathscr{H}\boldsymbol{x} \equiv \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \end{bmatrix} = \lambda \boldsymbol{x}, \tag{1.1}$$

where A and B are $n \times n$ real symmetric matrices. We refer to it a *linear response eigenvalue problem* (LREP). Any complex scalar λ and nonzero $2n$-dimensional column vector $\boldsymbol{x}$ that satisfy (1.1) are called an *eigenvalue* and its associated *eigenvector*, respectively, and correspondingly, $(\lambda, \boldsymbol{x})$ is called an *eigenpair*.

Our consideration of this problem is motivated by Casida's eigenvalue equations in [1–4]. In computational quantum chemistry and physics, the excitation states and response properties of molecules and clusters are predicted by the linear-response time-dependent density functional theory. The excitation energies and transition vectors (oscillator strengths) of molecular systems can be calculated by solving Casida's eigenvalue equations [1–3]. There has been a great deal of recent work on and interest in developing efficient numerical algorithms and simulation techniques for computing excitation responses of molecules and for material designs in energy science [5–12].

Let

$$\Gamma_0 = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix}, \ \Pi \equiv \Pi_{2n} = \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix}. \tag{1.2}$$

The matrix $\mathscr{H}$ in (1.1) satisfies

$$\Gamma_0\mathscr{H} = \begin{bmatrix} A & B \\ B & A \end{bmatrix} \text{ and } \mathscr{H}\Pi = -\Pi\mathscr{H}. \tag{1.3}$$

As a result of the second equation in (1.3), if $(\lambda, \boldsymbol{x})$ is an eigenpair of $\mathscr{H}$, i.e., $\mathscr{H}\boldsymbol{x} = \lambda\boldsymbol{x}$, then $(-\lambda, \Pi\boldsymbol{x})$ is also an eigenpair of $\mathscr{H}$, and if also $\lambda \notin \mathbb{R}$, then $\left(\bar{\lambda}, \bar{\boldsymbol{x}}\right)$ and $\left(-\bar{\lambda}, \Pi\bar{\boldsymbol{x}}\right)$ are eigenpairs of $\mathscr{H}$ as well, where $\bar{\lambda}$ is the complex conjugate of λ and $\bar{x}$ takes entrywise complex conjugation.

Previously in [5,6,13], LREP (1.1) was well-studied under the condition that $\Gamma_0\mathscr{H}$ is positive definite. For the case, all eigenvalues of $\mathscr{H}$ are real. Without the positive definite condition, the methods developed in [5,6,13] are not applicable.

Let $\mathbb{J}_n$ be the set of all $n \times n$ diagonal matrices with ± 1 on the diagonal and set

$$\boldsymbol{\Gamma}_{2n} = \{\text{diag}(J, -J) \ : \ J \in \mathbb{J}_n\}.$$

Note that $\Gamma_0 = \text{diag}(I_n, -I_n) \in \boldsymbol{\Gamma}_{2n}$. In this paper, we will study an eigenvalue problem for which the condition that $\Gamma_0\mathscr{H}$ is positive definite is no longer assumed and it in fact includes LREP (1.1) as a special case. Specifically, we will consider the following eigenvalue problem