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 $\Gamma_0 = \operatorname{diag}(I_n, -I_n)$. Based on newly introduced Γ-orthogonal transformations, the ΓQR algorithm preserves the $\boldsymbol{\Pi}^-$-symmetric structure of $\mathscr{H}$ throughout the whole process, which 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.

Keywords. $\boldsymbol{\Pi}^{\pm}$-matrix, Γ-orthogonality, structure preserving, ΓQR algorithm, linear response eigenvalue problem

AMS subject classifications. 15A18, 15A23, 65F15

1 Introduction

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

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

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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 [10, 15, 19, 22]. 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 [10, 15, 19]. 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 [2, 3, 12, 13, 17, 18, 20, 21].

Let

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

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 [2, 3, 23], 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 [2, 3, 23] are not applicable.

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

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

Note that $\Gamma_0 = \operatorname{diag}(I_n, -I_n) \in \boldsymbol{\Gamma}_{2n}$. 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

$$\mathscr{H}\boldsymbol{x} \equiv \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \boldsymbol{x} = \lambda\boldsymbol{x} \tag{1.4a}$$

with the structure property:

$$\boxed{\begin{array}{l}\text{there is a } \Gamma = \operatorname{diag}(J, -J) \in \boldsymbol{\Gamma}_{2n} \text{ with } J = \operatorname{diag}(\pm 1) \in \mathbb{J}_n \\ \text{such that } \Gamma\mathscr{H} = \begin{bmatrix} JA & JB \\ JB & JA \end{bmatrix} \text{ with } JA, JB \in \mathbb{R}^{n\times n} \text{ being} \\ \text{symmetric.}\end{array}} \tag{1.4b}$$

There are two reasons for considering this more general eigenvalue problem (1.4). The first reason is that this includes (1.1), with/without $\Gamma_0\mathscr{H}$ being positive definite, as a special case, and the second one is that the intermediate eigenvalue problems in our later iterative QR-like algorithm for solving (1.1) are of this kind, i.e., with $\Gamma \neq \Gamma_0$.

It can be verified that the second equation in (1.3), $\mathscr{H}\Pi = -\Pi\mathscr{H}$, still holds in the case of (1.4b). Therefore the same results about the eigenvalue pattern we mentioned for (1.1) remain valid. Namely, if $(\lambda, \boldsymbol{x})$ is an eigenpair, then $(-\lambda, \Pi\boldsymbol{x})$ is also an eigenpair, 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 as well. Another interesting result is about the Γ-orthogonality among the eigenvectors of $\mathscr{H}$. Specifically, for two eigenpairs $(\lambda, \boldsymbol{x})$ and $(\mu, \boldsymbol{y})$ of $\mathscr{H}$ if $\lambda \neq \bar{\mu}$, then it holds that $\boldsymbol{y}^{\mathrm{H}}\Gamma\boldsymbol{x} = 0$, where $\boldsymbol{y}^{\mathrm{H}}$ is the conjugate transpose of $\boldsymbol{y}$. This is because using (1.4b), we have

$$\lambda\boldsymbol{y}^{\mathrm{H}}\Gamma\boldsymbol{x} = \boldsymbol{y}^{\mathrm{H}}\Gamma\mathscr{H}\boldsymbol{x} = \boldsymbol{y}^{\mathrm{H}}\mathscr{H}^{\mathrm{H}}\Gamma\boldsymbol{x} = \bar{\mu}\boldsymbol{y}^{\mathrm{H}}\Gamma\boldsymbol{x}$$

and thus $(\lambda - \bar{\mu})\boldsymbol{y}^{\mathrm{H}}\Gamma\boldsymbol{x} = 0$ which yields $\boldsymbol{y}^{\mathrm{H}}\Gamma\boldsymbol{x} = 0$ when $\lambda \neq \bar{\mu}$.

The matrix $\mathscr{H}$ in (1.4) has some nice block structures. In fact, the eigenvalue problem (1.4) can be written as a special Hamiltonian eigenvalue problem

$$\begin{bmatrix} 0 & JM \\ JK & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \end{bmatrix} \text{ with } K = A - B, \quad M = A + B, \tag{1.5}$$

$\boldsymbol{y}_1 = \boldsymbol{x}_1 - \boldsymbol{x}_2$, and $\boldsymbol{y}_2 = \boldsymbol{x}_1 + \boldsymbol{x}_2$. There are several existing structure-preserving approaches [6, 8, 13, 16] can be applied to solve the eigenvalue problem (1.5).

(a) A periodic QR (PQR) algorithm with orthogonal transformations [16] can be used to solve the product eigenvalue problem $(JK)(JM)\boldsymbol{y}_2 = \lambda^2\boldsymbol{y}_2$ for (1.5). Here, the $n \times n$ block structure in (1.4) is exploited and the symmetry of the spectrum can be preserved. However, the symmetric structures of JA and JB are destroyed during the iterations.

(b) The KQZ algorithm [13] with orthogonal and Π-orthogonal transformations can be applied to solve $\mathscr{H}$ in (1.1). The block structure $\mathscr{H}\Pi = -\Pi\mathscr{H}$ is preserved during the KQZ iteration. The reduced matrices JA and JB in (1.4b) are no longer symmetric (tridiagonal), but only Hessenberg. It is mathematically different from the periodic QR algorithm, but they have the similar amount of computational costs.

(c) An HR process proposed by Brebner and Grad (BG) [6] is used to reduce the product eigenvalue problem $(JK)(JM)\boldsymbol{y}_2 = \lambda^2\boldsymbol{y}_2$ to a pseudosymmetric form $C\boldsymbol{z} = \lambda^2 J'\boldsymbol{z}$, where

C is symmetric tridiagonal and J' is the inertia sign-matrix of JK or JM. The tridiagonal pseudosymmetry in BG-algorithm are preserved during the HR iterations. The BG-algorithm has the similar amount of computational costs as our ΓQR algorithm. However, ill-conditioned K and M may cause the numerical instability of the BG-algorithm during constructing J'.

(d) The symplectic QR-like algorithm with symplectic transformations [8] can also be applied to solve the special Hamiltonian eigenvalue problem (1.5). The Hamiltonian matrix is reduced to a condensed Hamiltonian form $\begin{bmatrix} H_1 & H_3 \\ H2 & -H_1 \end{bmatrix}$ with H_1 and H_2 being diagonal and H_3 being symmetric triadiagonal, and then H_3-block will converge to a quasi-diagonal matrix. The symplectic QR-like algorithm does not really exploit the symmetry properties of JA and JB. Instability can occur when the symplectic Gaussian elimination matrices at some steps have larger condition numbers. This phenomenon can not be avoided because to maintain the Hamiltonian structure only the Gaussian elimination without pivot is allowed. Furthermore, the symplectic matrices Q in the symplectic QR-like algorithm satisfy $Q^\top JQ = J$, where $J = \mathit{\Gamma}_0 \mathit{\Pi}$. The $\mathit{\Gamma}$-orthogonal matrices Q in our newly developed ΓQR algorithm (later) satisfy $Q\mathit{\Pi} = \mathit{\Pi} Q$ and $Q^\top \mathit{\Gamma} Q = \mathit{\Gamma}'$ with $\mathit{\Gamma}, \mathit{\Gamma}' \in \boldsymbol{\Gamma}_{2n}$. The intersection of these two classes is the set of matrices Q that satisfy $Q\mathit{\Pi} = \mathit{\Pi} Q$ and $Q^\top \mathit{\Gamma} Q = \mathit{\Gamma}'$ which is much smaller than two transformation sets.

(e) The Hamiltonian QR-algorithm with symplectic orthogonal transformations proposed by [9] is only suitable for a very special Hamiltonian eigenvalue problem such as in (1.1) or (1.5) with rank(B), rank(K), or rank(M) being one. one of rank(B), rank(K), and rank(M) is one?

The HR algorithm proposed in [7] is a pioneering work for solving the eigenvalue problem of an $n \times n$ matrix $\mathscr{A}$ having the property that there exists a so-called *pseudo-orthogonal* matrix H in the sense that $H^\top JH = J'$ for some $J = \mathrm{diag}(\pm 1)$ and $J' = \mathrm{diag}(\pm 1)$ having the same inertia such that $H^{-1}\mathscr{A} H = R$ is upper triangular. In light of the HR algorithm in [7], the main task of this paper is to develop iterative ΓQR algorithms for solving (1.4), while exploiting the inherent structures in $\mathscr{H}$ and $\mathit{\Gamma}$ for better numerical efficiency, based on $(\mathit{\Gamma}, \mathit{\Gamma}')$-orthogonal transformations with $\mathit{\Gamma}, \mathit{\Gamma}' \in \boldsymbol{\Gamma}_{2n}$ to be defined in Section 2. The transformations preserve the symmetry structures in $\mathit{\Gamma}\mathscr{H}$ and the diagonal structure of $\mathit{\Gamma}$. Throughout this paper, we assume that $\mathscr{H}$ is nonsingular, and thus 0 is not an eigenvalue of (1.1).

The rest of this paper is organized as follows. In Section 2, we introduce some basic definitions and state their immediately implied properties. In Section 3, we first give two kinds of $\mathit{\Gamma}$-orthogonal transformations, and then prove existence and uniqueness of the ΓQR factorization and propose an algorithm to compute the factorization for a given matrix G with $G\mathit{\Pi} = -\mathit{\Pi} G$. In Section 4, we present the $\boldsymbol{\Pi}^-$-upper Hessenberg reduction/tridiagonalization and prove the implicit $\mathit{\Gamma}$-orthognality theorem of a $\boldsymbol{\Pi}^-$-matrix G. In Section 5, we develop ΓQR algorithms for computing all eigenpairs of $\mathscr{H}$ and analyze their convergence with the goal of an efficient implicit multi-shift ΓQR algorithm. Numerical results of the ΓQR algorithm compared to the other existing algorithm are shown in Section 6. Finally, some conclusions are drawn in Section 7.

Notation. $\mathbb{C}^{n\times m}$ is the set of all $n\times m$ complex matrices with real entries, $\mathbb{R}^n = \mathbb{R}^{n\times 1}$, and $\mathbb{R} = \mathbb{R}^1$. We denote by I_n and $\mathbf{0}_{m\times n}(\mathbf{0}_m)$ the $n\times n$ identity matrix and $m\times n$ ($m\times m$) zero matrix, respectively, and their subscripts may be dropped if their sizes can be read from the context. $\mathit{\Gamma}_0$ and $\mathit{\Pi}_{2n}$ are reserved as given by (1.2), and often the subscript to $\mathit{\Pi}_{2n}$ is dropped, too, when no confusion is possible. The jth column of the identity matrix I is $\boldsymbol{e}_j$ whose size will be determined by the context. We shall also adopt MATLAB-like convention to access the entries of vectors and matrices. Let $i:j$ be the set of integers from i to j inclusive. For a vector $\boldsymbol{u}$ and a matrix X, $\boldsymbol{u}_{(j)}$ is the jth entry of $\boldsymbol{u}$ and $X_{(i,j)}$ is the (i,j)th entry of X; $X_{(\mathbb{I}_1,\mathbb{I}_2)}$ is the submatrix of X consist of intersections of all rows $i\in\mathbb{I}_1$ and all columns $j\in\mathbb{I}_2$; $X^\top$ is the transpose of X. We denote by $\mathrm{eig}(A)$ the spectrum of matrix A, and $\mathrm{diag}(X,Y)$ is the 2-by-2 block-diagonal matrix with diagonal blocks X and Y.

2 Definitions and Preliminaries

In this section, we introduce several kinds of matrix classes and their essential properties. Recall $\mathit{\Pi}_{2n}$ defined in (1.2).

Definition 2.1. Let $G\in\mathbb{R}^{2n\times 2m}$ with $m\le n$. G is called a $\boldsymbol{\mathit{\Pi}}^{\pm}$*-matrix* if i.e.,

$$G\mathit{\Pi}_{2m} = \pm\mathit{\Pi}_{2n}G, \text{ i.e., } G = \begin{bmatrix} G_1 & G_2 \\ \pm G_2 & \pm G_1 \end{bmatrix} \text{ with } G_1,\ G_2\in\mathbb{R}^{n\times m}. \tag{2.1}$$

Denote by $\boldsymbol{\mathit{\Pi}}^{\pm}_{2n\times 2m}$ the set of all $2n\times 2m$ $\boldsymbol{\mathit{\Pi}}^{\pm}$-matrices, and $\boldsymbol{\mathit{\Pi}}^{\pm}_{2n} := \boldsymbol{\mathit{\Pi}}^{\pm}_{2n\times 2n}$ for short.

In this definition and those below, to save space and avoid repetitions, we often pack two statements into one: one for $\boldsymbol{\mathit{\Pi}}^{+}$-matrix and the other for $\boldsymbol{\mathit{\Pi}}^{-}$-matrix. In the same spirit, in definitions/statements in the rest of this paper, any of them with phrases in parentheses is understood that the phrases can be used to replace the phrases immediately before for another definition/statement.

We say a matrix X, possibly nonsquare, is *upper Hessenberg* if $X_{(i,j)} = 0$ for $i > j+1$, *upper triangular* if $X_{(i,j)} = 0$ for $i > j$, and diagonal if $X_{(i,j)} = 0$ for $i \ne j$. This is consistent with the standard definitions of upper Hessenberg, upper triangular, and diagonal matrices which are usually for square matrices.

A *quasi-upper triangular matrix* means that it is a block upper triangular matrix with diagonal blocks being 1×1 or 2×2. Similarly, a *quasi-diagonal matrix* means that it is a block diagonal matrix with diagonal blocks being 1×1 or 2×2.

Definition 2.2. Let $G \in \boldsymbol{\Pi}^-_{2n\times 2m}$ as in (2.1).

1. G is *$\boldsymbol{\Pi}^-$-upper Hessenberg* if G_1 is upper Hessenberg and G_2 is upper triangular.

   G is *unreduced $\boldsymbol{\Pi}^-$-upper Hessenberg* if G_1 is unreduced upper Hessenberg.

2. G is *$\boldsymbol{\Pi}^-$-upper ($\boldsymbol{\Pi}^-$-quasi-upper) triangular* if G_1 is upper (quasi-upper) triangular and G_2 is strictly upper triangular.

   Denote by $\mathbb{U}^-_{2n\times 2m}$ ($\mathrm{q}\mathbb{U}^-_{2n\times 2m}$) the set of all $2n \times 2m$ $\boldsymbol{\Pi}^-$-upper ($\boldsymbol{\Pi}^-$-quasi-upper) triangular matrices, and write, for short, $\mathbb{U}^-_{2n} := \mathbb{U}^-_{2n\times 2n}$ and $\mathrm{q}\mathbb{U}^-_{2n} := \mathrm{q}\mathbb{U}^-_{2n\times 2n}$.

3. G is *$\boldsymbol{\Pi}^-$-diagonal ($\boldsymbol{\Pi}^-$-quasi-diagonal)* if G_1 is diagonal (quasi-diagonal) and G_2 is diagonal.

   Denote by $\mathbb{D}^-_{2n\times 2m}$ ($\mathrm{q}\mathbb{D}^-_{2n\times 2m}$) the set of all $2n \times 2n$ $\boldsymbol{\Pi}^-$-diagonal ($\boldsymbol{\Pi}^-$-quasi-diagonal) matrices, and write, for short, $\mathbb{D}^-_{2n} := \mathbb{D}^-_{2n\times 2n}$ and $\mathrm{q}\mathbb{D}^-_{2n} := \mathrm{q}\mathbb{D}^-_{2n\times 2n}$.

Definition 2.3. 1. Let $G \in \boldsymbol{\Pi}^+_{2n}$ as in (2.1). G is *$\boldsymbol{\Pi}^+$-symmetric ($\boldsymbol{\Pi}^+$-sym-tridiagonal)*, if G_1 is symmetric (symmetric tridiagonal) and G_2 is symmetric (diagonal).

2. Let $G \in \boldsymbol{\Pi}^-_{2n}$ as in (2.1). G is *$\boldsymbol{\Pi}^-$-symmetric ($\boldsymbol{\Pi}^-$-sym-tridiagonal)* with respect to $\Gamma \in \boldsymbol{\Gamma}_{2n}$ if ΓG is $\boldsymbol{\Pi}^+$-symmetric ($\boldsymbol{\Pi}^+$-sym-tridiagonal).

3. G is *unreduced $\boldsymbol{\Pi}^\pm$-sym-tridiagonal* if it is $\boldsymbol{\Pi}^\pm$-sym-tridiagonal and G_1 is unreduced.

The following propositions are direct consequences of Definitions 2.1 – 2.3 and are rather straightforward to verify.

Proposition 2.1. (i) *$G \in \boldsymbol{\Pi}^\pm_{2n\times 2m}$ if and only if $\Gamma G \in \boldsymbol{\Pi}^\mp_{2n\times 2m}$ and $G\Gamma' \in \boldsymbol{\Pi}^\mp_{2n\times 2m}$ for any $\Gamma \in \boldsymbol{\Gamma}_{2n}$ and $\Gamma' \in \boldsymbol{\Gamma}_{2m}$.*

(ii) *The inverse of a $\boldsymbol{\Pi}^\pm$-(upper triangular) matrix is still a $\boldsymbol{\Pi}^\pm$-(upper triangular) matrix.*

(iii) *The product $\widetilde{G}G$ of two $2n \times 2n$ matrices $\widetilde{G}$ and G in their respective categories belongs to the one as listed in the following table.*

don't need the other table? keep it anyway?

$\widetilde{G}$ \ G	$\boldsymbol{\Pi}^+$	$\boldsymbol{\Pi}^-$
$\boldsymbol{\Pi}^+$	$\boldsymbol{\Pi}^+$	$\boldsymbol{\Pi}^-$
$\boldsymbol{\Pi}^-$	$\boldsymbol{\Pi}^-$	$\boldsymbol{\Pi}^+$

Proposition 2.2. *Let $G \in \boldsymbol{\Pi}^-_{2n}$. Then G has $2n$ eigenvalues, appearing in pairs $(\lambda, -\lambda)$ for real or purely imaginary eigenvalues λ and in quadruples $(\pm\lambda, \pm\bar{\lambda})$ for complex eigenvalues λ.*

Proof. By Definition 2.1, it holds that

$$\det(G - \lambda I) = \det(\mathit{\Pi} G - \lambda \mathit{\Pi}) = \det(G\mathit{\Pi} + \lambda \mathit{\Pi}) = \det(G + \lambda I) = 0.$$

The assertion follows immediately. □

Definition 2.4. $Q \in \boldsymbol{\mathit{\Pi}}^+_{2n\times 2m}$ is $\mathit{\Gamma}$-*orthogonal* with respect to $\mathit{\Gamma} \in \boldsymbol{\mathit{\Gamma}}_{2n}$ if $\mathit{\Gamma}' := Q^\top \mathit{\Gamma} Q \in \boldsymbol{\mathit{\Gamma}}_{2m}$. Denote by $\mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n\times 2m}$ the set of all $2n \times 2m$ $\mathit{\Gamma}$-orthogonal matrices, and $\mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n} := \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n\times 2n}$ for short.

Often, for short, we may say $Q \in \boldsymbol{\mathit{\Pi}}^+_{2n\times 2m}$ is $\mathit{\Gamma}$-orthogonal, by which we mean there is $\mathit{\Gamma} \in \boldsymbol{\mathit{\Gamma}}_{2n}$ that has the requirement of the definition satisfied. Similarly, we may simply say Q is $\mathit{\Gamma}$-orthogonal. The same understanding applies to the expression $Q \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n\times 2m}$.

Proposition 2.3. *Let $Q_i \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n}$ with respect to $\mathit{\Gamma}_i \in \boldsymbol{\mathit{\Gamma}}_{2n}$ for $i = 1, 2$, and suppose $\mathit{\Gamma}_2 = Q_1^\top \mathit{\Gamma}_1 Q_1$.*

(i) *$Q_1 Q_2 \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n}$ with respect to $\mathit{\Gamma}_1$.*

(ii) *Q_i is nonsingular and $Q_i^{-1} = \mathit{\Gamma}_{i+1} Q_i^\top \mathit{\Gamma}_i$, where $\mathit{\Gamma}_3 := Q_2^\top \mathit{\Gamma}_2 Q_2$.*

(iii) *If also $Q_i \in \mathbb{U}^+_{2n}$, then $Q_i = J_i \oplus J_i$ for some $J_i \in \mathbb{J}_n$.*

Proof. Items (i) and (ii) follow from Definition 2.4 directly. For item (iii), $Q_i^{-1} \in \mathbb{U}^+_{2n}$ by Proposition 2.1(ii). On the other hand, by item (ii), $Q_i^{-1} = \mathit{\Gamma}_{i+1} Q_i^\top \mathit{\Gamma}_i$ which is $\boldsymbol{\mathit{\Pi}}^+$-lower triangular. This implies that $Q_i = J_i \oplus J_i$ for some $J_i \in \mathbb{J}_n$, completing the proof of item (iii). □

3 ΓQR Factorization

Definition 3.1. $G = QR$ is called a ΓQR *factorization* of $G \in \boldsymbol{\mathit{\Pi}}^-_{2n\times 2m}$ with respect to $\mathit{\Gamma} \in \boldsymbol{\mathit{\Gamma}}_{2n}$ if $R \in \mathbb{U}^-_{2n\times 2m}$ and $Q \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n}$ with respect to $\mathit{\Gamma}$ or if $R \in \mathbb{U}^-_{2m}$ and $Q \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n\times 2m}$ with respect to $\mathit{\Gamma}$.

The case when $R \in \mathbb{U}^-_{2m}$ and $Q \in \mathbb{O}^{\boldsymbol{\mathit{\Gamma}}}_{2n\times 2m}$ with respect to $\mathit{\Gamma}$ in this definition corresponds to the so-called *skinny* QR factorization in numerical linear algebra.

Definition 3.2. Let $M = \begin{bmatrix} M_1 & M_2 \\ -M_2 & -M_1 \end{bmatrix} \in \boldsymbol{\mathit{\Pi}}^-_{2n}$, and set

$$M_{1i} = (M_1)_{(1:i,1:i)}, \quad M_{2i} = (M_2)_{(1:i,1:i)}.$$

$\begin{bmatrix} M_{1i} & M_{2i} \\ -M_{2i} & -M_{1i} \end{bmatrix}$ is called the ith $\boldsymbol{\mathit{\Pi}}^-$-*leading principal submatrix* of M and its determinant is called the ith $\boldsymbol{\mathit{\Pi}}^-$-*leading principal minor* of M.

The next theorem shows that almost every $\boldsymbol{\Pi}^-$-matrix $G \in \boldsymbol{\Pi}^-_{2n\times 2m}$ has a ΓQR factorization with respect to a given $\Gamma \in \boldsymbol{\Gamma}_{2n}$ and the factorization is unique if it is required that the top-left quarter of the R-factor has positive diagonal entries.

Theorem 3.1. *Suppose that $G \in \boldsymbol{\Pi}^-_{2n\times 2m} (m \le n)$ has full column rank and $\Gamma \in \boldsymbol{\Gamma}_{2n}$.*

(i) *If $G = QR = \widetilde{Q}\widetilde{R}$ (with $Q, \widetilde{Q} \in \mathbb{O}^{\boldsymbol{\Gamma}}_{2n\times 2m}$ and $R, \widetilde{R} \in \mathbb{U}^-_{2m}$) are two* ΓQR *factorizations of G with respect to Γ, then*

$$\widetilde{Q}^\top \Gamma \widetilde{Q} = Q^\top \Gamma Q \in \boldsymbol{\Gamma}_{2m}$$

and there is a $\boldsymbol{\Pi}^+$-diagonal matrix $D = J \oplus J$ with $J \in \mathbb{J}_m$ such that $\widetilde{Q} = QD$ and $\widetilde{R} = DR$. In particular, if the top-left quarters of R and $\widetilde{R}$ have positive diagonal entries, then $D = I_{2m}$, $Q = \widetilde{Q}$, and $R = \widetilde{R}$.

(ii) *G has a* ΓQR *factorization with respect to Γ if and only if no $\boldsymbol{\Pi}^-$-leading principal minor of $G^\top \Gamma G$ vanishes.*

Proof. We first prove item (i). Let $\Gamma' = Q^\top \Gamma Q$ and $\widetilde{\Gamma}' = \widetilde{Q}^\top \Gamma \widetilde{Q}$. From the assumption we have

$$\Gamma' R = Q^\top \Gamma Q R = Q^\top \Gamma \widetilde{Q}\widetilde{R} \quad \Rightarrow \quad Q^\top \Gamma \widetilde{Q} = \Gamma' R \widetilde{R}^{-1}.$$

Similarly, $\widetilde{Q}^\top \Gamma Q = \widetilde{\Gamma}' \widetilde{R} R^{-1}$. Therefore

$$\widetilde{\Gamma}' \widetilde{R} R^{-1} = \widetilde{Q}^\top \Gamma Q = (Q^\top \Gamma \widetilde{Q})^\top = (\Gamma' R \widetilde{R}^{-1})^\top = \widetilde{R}^{-\top} R^\top \Gamma'. \tag{3.1}$$

Because $\widetilde{\Gamma}' \widetilde{R} R^{-1} \in \mathbb{U}^-_{2m}$ and at the same time $\widetilde{R}^{-\top} R^\top \Gamma'$ is $\boldsymbol{\Pi}^-$-lower triangular, we conclude that $\widetilde{R} R^{-1}$ and $\widetilde{R}^{-\top} R^\top$ must be diagonal. Set

$$D = \widetilde{R} R^{-1} \in \boldsymbol{\Pi}^+_{2m} \tag{3.2}$$

which implies $\widetilde{R}^{-\top} R^\top = (\widetilde{R} R^{-1})^{-\top} = D^{-1}$. Thus, from (3.1) and (3.2), we have $\widetilde{\Gamma}' D = \widetilde{Q}^\top \Gamma Q$ and $\Gamma' D^{-1} = Q^\top \Gamma \widetilde{Q}$. This implies $\Gamma' = D \widetilde{\Gamma}' D$, and thus

$$D^2 = I_{2m}, \quad \Gamma' = \widetilde{\Gamma}' \in \boldsymbol{\Gamma}_{2m}.$$

So $D = \mathrm{diag}(J, -J)$ for some $J \in \mathbb{J}_m$ and $\widetilde{R} = DR$. Furthermore, since $G = QR = \widetilde{Q}\widetilde{R}$ has full column rank, it follows that $\widetilde{Q} = QD$.

Now if also the top-left quarters of R and $\widetilde{R}$ have positive diagonal entries, then $\widetilde{R} = DR$ implies $D = I_{2m}$, as expected.

Next we prove item (ii).

Necessity. Let P be the permutation matrix

$$P = [\boldsymbol{e}_1, \boldsymbol{e}_3, \cdots, \boldsymbol{e}_{2m-1} \,|\, \boldsymbol{e}_2, \boldsymbol{e}_4, \cdots, \boldsymbol{e}_{2m}] \in \mathbb{R}^{2m\times 2m}. \tag{3.3}$$

Suppose that $G = QR$ is a ΓQR factorization with respect to $\mathit{\Gamma}$, and let $\mathit{\Gamma}' = Q^\top \mathit{\Gamma} Q$. Then

$$P^\top G^\top \mathit{\Gamma} G P = (P^\top R^\top P)(P^\top \mathit{\Gamma}' P)(P^\top R P) =: R_{\mathbf{p}}^\top \mathit{\Gamma}'_{\mathbf{p}} R_{\mathbf{p}},$$

where $R_{\mathbf{p}} = P^\top R P$ is upper triangular and $\mathit{\Gamma}'_{\mathbf{p}} = P^\top \mathit{\Gamma}' P$ is diagonal, as in

$$R_{\mathbf{p}} = \begin{bmatrix} R_{11} & \cdots & R_{1m} \\ \vdots & \ddots & \vdots \\ 0 & \cdots & R_{mm} \end{bmatrix}, \quad \mathit{\Gamma}'_{\mathbf{p}} = \begin{bmatrix} \mathit{\Gamma}'_{11} & & 0 \\ & \ddots & \\ 0 & & \mathit{\Gamma}'_{mm} \end{bmatrix} \tag{3.4}$$

with $R_{ij} \in \boldsymbol{\mathit{\Pi}}_2^-$, $R_{ii} = \begin{bmatrix} d_i & 0 \\ 0 & -d_i \end{bmatrix}$, and $\mathit{\Gamma}'_{ii} \in \boldsymbol{\mathit{\Gamma}}_2$ for $i, j = 1, \cdots, m$. Since G has full column rank, it follows that $\det(R_{ii}) \neq 0$ for $i = 1, \cdots, m$. Therefore, there is no leading principal minor of $P^\top G^\top \mathit{\Gamma} G P$ of even order vanishes, i.e., no $\boldsymbol{\mathit{\Pi}}^-$-leading principal minor of $G^\top \mathit{\Gamma} G$ vanishes.

Sufficiency. Suppose that $G \in \boldsymbol{\mathit{\Pi}}_{2n\times 2m}^-$ and no $\boldsymbol{\mathit{\Pi}}^-$-leading principal minor of $M := G^\top \mathit{\Gamma} G$ vanishes. Then there is an LU factorization of $M_{\mathbf{p}} := P^\top M P$: $M_{\mathbf{p}} = L_{\mathbf{p}} \widehat{R}_{\mathbf{p}}$ with nonsingular

$$L_{\mathbf{p}} = \begin{bmatrix} I_2 & & & 0 \\ L_{21} & I_2 & & \\ \vdots & \ddots & \ddots & \\ L_{m1} & \cdots & L_{m,m-1} & I_2 \end{bmatrix}, \quad \widehat{R}_{\mathbf{p}} = \begin{bmatrix} \widehat{R}_{11} & \cdots & \widehat{R}_{1m} \\ & \ddots & \vdots \\ 0 & & \widehat{R}_{mm} \end{bmatrix}, \tag{3.5}$$

where $L_{ij} \in \boldsymbol{\mathit{\Pi}}_2^+$ and $\widehat{R}_{ij} \in \boldsymbol{\mathit{\Pi}}_2^-$. Decompose $\widehat{R}_{\mathbf{p}}$ as

$$\widehat{R}_{\mathbf{p}} = \begin{bmatrix} \widehat{R}_{11} & & 0 \\ & \ddots & \\ 0 & & \widehat{R}_{mm} \end{bmatrix} \begin{bmatrix} I_2 & R_{12} & \cdots & R_{1m} \\ & \ddots & \ddots & \vdots \\ & & \ddots & R_{m-1,m} \\ & & & I_2 \end{bmatrix} =: \widehat{D}_{\mathbf{p}} R_{\mathbf{p}} \tag{3.6}$$

with $R_{ij} = \widehat{R}_{ii}^{-1} \widehat{R}_{ij} \in \boldsymbol{\mathit{\Pi}}_2^+$. Then we have

$$M_{\mathbf{p}} = L_{\mathbf{p}} \widehat{R}_{\mathbf{p}} = L_{\mathbf{p}} \widehat{D}_{\mathbf{p}} R_{\mathbf{p}} = R_{\mathbf{p}}^\top \widehat{D}_{\mathbf{p}}^\top L_{\mathbf{p}}^\top = M_{\mathbf{p}}^\top. \tag{3.7}$$

The uniqueness of the LU factorization implies that $L_{\mathbf{p}}^\top = R_{\mathbf{p}}$. Since $M_{\mathbf{p}}$ is symmetric, it follows that $\widehat{D}_{\mathbf{p}} = \operatorname{diag}(\{\widehat{R}_{ii}\}_{i=1}^m)$ is symmetric. Because $\widehat{R}_{ii} \in \boldsymbol{\mathit{\Pi}}_2^-$, $\widehat{R}_{ii}$ must be of the form $\widehat{R}_{ii} = \begin{bmatrix} d_i & 0 \\ 0 & -d_i \end{bmatrix}$ for $i = 1, \cdots, m$. Write

$$\widehat{R}_{ii} = \begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix} \begin{bmatrix} \operatorname{sgn}(d_i) & 0 \\ 0 & -\operatorname{sgn}(d_i) \end{bmatrix} \begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix}$$

and denote

$$D_{\mathbf{p}}^{1/2} = \mathrm{diag}(\left\{\begin{bmatrix} \sqrt{|d_i|} & 0 \\ 0 & \sqrt{|d_i|} \end{bmatrix}\right\}_{i=1}^{m}), \quad \Gamma'_{\mathbf{p}} = \mathrm{diag}(\left\{\begin{bmatrix} \mathrm{sgn}(d_i) & 0 \\ 0 & -\mathrm{sgn}(d_i) \end{bmatrix}\right\}_{i=1}^{m}). \tag{3.8}$$

From (3.7) and (3.8) we have

$$G^\top \Gamma G = PM_{\mathbf{p}}P^\top = (PL_{\mathbf{p}}D_{\mathbf{p}}^{1/2}P^\top)(P\Gamma'_{\mathbf{p}}P^\top)(PD_{\mathbf{p}}^{1/2}L_{\mathbf{p}}^\top P^\top) =: R^\top \Gamma' R, \tag{3.9}$$

where $R = PD_{\mathbf{p}}^{1/2}L_{\mathbf{p}}^\top P^\top \in \mathbb{U}_{2m}^{+}$ and $\Gamma' = P\Gamma'_{\mathbf{p}}P^\top$. Let

$$Q_- := GR^{-1}\Gamma' \in \boldsymbol{\Pi}_{2n\times 2m}^{+}. \tag{3.10}$$

With the help of (3.9), it can be verified that

$$Q_-^\top \Gamma Q_- = (\Gamma' R^{-\top}G^\top)\Gamma(GR^{-1}\Gamma') = \Gamma' R^{-\top}(R^\top \Gamma' R)R^{-1}\Gamma' = \Gamma'$$

which says $Q_- \in \mathbb{O}_{2n\times 2m}^{\boldsymbol{\Gamma}}$. Therefore

$$G = (GR^{-1}\Gamma')(\Gamma' R) =: Q_- R_- \quad \text{with} \quad R_- \in \mathbb{U}_{2m}^{-} \tag{3.11}$$

to give $G = QR$, a ΓQR factorization. □

Our goal in this paper is to develop a structure-preserving QR-like algorithm to compute all eigenvalues of $\mathscr{H} \in \boldsymbol{\Pi}_{2n}^{-}$. The basic idea is to calculate a sequence of Γ-orthogonal matrices $\{Q_i\}$, based on a ΓQR factorization, such that

$$\mathscr{H}_{i+1} = Q_i^{-1}\mathscr{H}_i Q_i, \quad Q_i^\top \Gamma_i Q_i = \Gamma_{i+1} \quad \text{for } i = 1, 2, \ldots,$$

where initially $\mathscr{H}_0 = \mathscr{H}$. For this purpose, at first, we introduce two elementary Γ-orthogonal transformations which will be used to zero out a specific entry of a vector. Specifically, given $\Gamma \in \boldsymbol{\Gamma}_{2n}$ and $\boldsymbol{u} \in \mathbb{R}^{2n}$, we seek $Q \in \mathbb{O}_{2n}^{\boldsymbol{\Gamma}}$ to zero out some portion of $\boldsymbol{u}$. Two different kinds of matrices Q will be used to deal with all possible scenarios that will occur in computing the ΓQR factorizations in Algorithm 3.1 later.

Let $\boldsymbol{a} \in \mathbb{R}^k$ $(1 \le k \le n)$, $J \equiv \mathrm{diag}(\jmath_1, ..., \jmath_k) \in \mathbb{J}_k$. Assume that $\boldsymbol{a}^\top J\boldsymbol{a} \neq 0$. Let P_a be a permutation which is chosen by interchanging row 1 and row r $(2 \le r \le k)$ of J such that $\hat{\jmath}_1\boldsymbol{a}^\top J\boldsymbol{a} = \hat{\jmath}_1\hat{\boldsymbol{a}}^\top \widehat{J}\hat{\boldsymbol{a}} > 0$, where $\hat{\boldsymbol{a}} = P_a\boldsymbol{a}$ and $\widehat{J} = P_a J P_a = \mathrm{diag}(\hat{\jmath}_1, ..., \hat{\jmath}_k)$. A Householder-like transformation is proposed by [7] to zero out the elements of $\hat{\boldsymbol{a}}_{(2:k)}$ as follows. Let

$$H(\boldsymbol{a})^{-1} = I - \frac{\hat{\jmath}_1}{\beta}(\hat{\boldsymbol{a}} - \alpha e_1)(\hat{\boldsymbol{a}} - \alpha e_1)^\top \widehat{J}, \quad \widehat{H}(\boldsymbol{a})^{-1} = H(\boldsymbol{a})^{-1}P_a, \tag{3.12a}$$

where $\alpha = -\mathrm{sign}(\hat{\boldsymbol{a}}_{(1)})\sqrt{\hat{\jmath}_1\hat{\boldsymbol{a}}^\top \widehat{J}\hat{\boldsymbol{a}}}$ and $\beta = \alpha[\alpha - \hat{\boldsymbol{a}}_{(1)}]$. Then it can be verified that

$$\widehat{H}(\boldsymbol{a})^{-1}\boldsymbol{a} = [H(\boldsymbol{a})^{-1}P_a]\boldsymbol{a} = H(\boldsymbol{a})^{-1}\hat{\boldsymbol{a}} = \alpha e_1, \quad \widehat{H}(\boldsymbol{a})^\top J\widehat{H}(\boldsymbol{a}) = \widehat{J}. \tag{3.12b}$$

Hyp_Householder (hyperbolic Householder) transformation: Suppose $1 \le \ell < m \le n$, $\boldsymbol{u} \in \mathbb{R}^{2n}$ and $\Gamma = \operatorname{diag}(\gamma_1, \dots, \gamma_n, -\gamma_1, \dots, -\gamma_n) \in \boldsymbol{\Gamma}_{2n}$. There are two cases:

Case 1. $\boldsymbol{a} \leftarrow \boldsymbol{u}_{(\ell':m')}$ with $\ell' = n + \ell$ and $m' = n + m$, $J = \operatorname{diag}(\gamma_\ell, \dots, \gamma_m)$;

Case 2. $\boldsymbol{a} \leftarrow \boldsymbol{u}_{(\ell:m)}$, $J = \operatorname{diag}(\gamma_\ell, \dots, \gamma_m)$.

Using (3.12) we construct a hyperbolic Householder Γ-orthogonal transformation Q with respect to Γ through its inverse by

$\mathcal{Q}_h(\ell' : m'; \boldsymbol{u})$ not defined yet

$$Q^{-1} = \begin{cases} \mathcal{Q}_h(\ell' : m'; \boldsymbol{u}), & \text{case 1;} \\ \mathcal{Q}_h(\ell : m; \boldsymbol{u}), & \text{case 2,} \end{cases}$$
$$= \operatorname{diag}(I_{\ell-1}, \hat{H}(a)^{-1}, I_{n-m}, I_{\ell-1}, \hat{H}(a)^{-1}, I_{n-m}). \tag{3.13}$$

Then it holds that

$$Q^{-1}\boldsymbol{u} = \hat{\boldsymbol{u}} \text{ with } \begin{cases} \hat{\boldsymbol{u}}_{(\ell'+1:m')} = 0, & \text{case 1;} \\ \hat{\boldsymbol{u}}_{(\ell+1:m)} = 0, & \text{case 2,} \end{cases} \tag{3.14}$$

and $Q^\top \Gamma Q = \Gamma'$, where $\Gamma' = (\gamma'_1, \cdots, \gamma'_n, -\gamma'_1, \cdots, -\gamma'_n)$ is given by

$$\begin{cases} \gamma'_s = \gamma_s\,, & s = 1, \cdots, \ell - 1 \text{ and } m + 1, \cdots, n, \\ \gamma'_{s+\ell-1} = \widehat{j}_s\,, & s = 1, \cdots, m - \ell + 1. \end{cases} \tag{3.15}$$

Hyp_Givens (hyperbolic Givens) transformation: Suppose $1 \le \ell \le n$, $\boldsymbol{u} \in \mathbb{R}^{2n}$ and $\Gamma = \operatorname{diag}(\gamma_1, \cdots, \gamma_n, -\gamma_1, \cdots, -\gamma_n) \in \mathbf{\Gamma_{2n}}$. Let $\alpha \leftarrow \boldsymbol{u}_{(\ell)}$, $\beta \leftarrow \boldsymbol{u}_{(n+\ell)}$. Define

$$\begin{cases} c = \frac{1}{\sqrt{1-r^2}}, s = \frac{r}{\sqrt{1-r^2}} \text{ with } r = \frac{\beta}{\alpha}, \text{ if } |\alpha| > |\beta|\,, \\ c = \frac{r}{\sqrt{1-r^2}}, s = \frac{1}{\sqrt{1-r^2}} \text{ with } r = \frac{\alpha}{\beta}, \text{ if } |\alpha| < |\beta|\,. \end{cases} \tag{3.16}$$

We construct a hyperbolic Givens Γ-orthogonal transformation with respect to Γ through its inverse by

$$Q^{-1} = \mathcal{Q}_g(\ell; \alpha; \beta) = \begin{bmatrix} C & S \\ S & C \end{bmatrix} \in \Pi^+_{2n}, \tag{3.17}$$

where C is obtained from I_n by resetting $C_{(\ell,\ell)} = c$ and S from $O_{n\times n}$ by resetting $S_{(\ell,\ell)} = -s$. Then we have

$$Q^{-1}\boldsymbol{u} = \hat{\boldsymbol{u}} \quad \text{with} \quad \hat{\boldsymbol{u}}_{(n+\ell)} = 0,$$

Algorithm 3.1 ΓQR factorization

Input: $G \in \boldsymbol{\Pi}^{-}_{2n\times 2m}$, $\Gamma = \mathrm{diag}(J, -J) \in \boldsymbol{\Gamma}_{2n}$ with $J = \mathrm{diag}(\gamma_1, \cdots, \gamma_n)$, $n' \leftarrow 2n$;

Output: $Q \in \mathbb{O}^{\boldsymbol{\Gamma}}_{2n}$ with respect to Γ, $\Gamma' = Q^\top \Gamma Q \in \mathbb{J}_n$, and $R \in \mathbb{U}^{-}_{2m}$ such that $G = QR$;

1: $Q \leftarrow I_{2n}$, $\Gamma_{\mathrm{sav}} \leftarrow \Gamma$;
2: **for** $\ell = 1 : m$ **do**
3: $\quad \ell' \leftarrow n + \ell$, $\boldsymbol{u} \leftarrow G_{(:,\ell)}$;
4: $\quad$ compute Hyp_Householder Γ-orthogonal transformation: $\widetilde{Q}^{-1} = \mathcal{Q}_h(\ell' : n'; \boldsymbol{u})$ with respect to Γ (by (3.13));
5: $\quad Q \leftarrow Q\widetilde{Q}$, $G \leftarrow \widetilde{Q}^{-1}G$, $\Gamma \leftarrow -\Gamma'$ (by (3.15));
6: $\quad \alpha \leftarrow G_{(\ell,\ell)}$, $\beta \leftarrow G_{(\ell',\ell)}$;
7: $\quad$ compute Hyp_Givens Γ-orthogonal transformation: $\widetilde{Q}^{-1} = \mathcal{Q}_g(\ell; \alpha, \beta)$ with respect to Γ (by (3.17));
8: $\quad Q \leftarrow Q\widetilde{Q}$, $G \leftarrow \widetilde{Q}^{-1}G$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
9: $\quad \boldsymbol{u} \leftarrow G_{(:,\ell)}$;
10: $\quad$ compute Hyp_Householder Γ-orthogonal transformation: $\widetilde{Q}^{-1} = \mathcal{Q}_h(\ell : n; \boldsymbol{u})$ with respect to Γ (by (3.13));
11: $\quad Q \leftarrow Q\widetilde{Q}$, $G \leftarrow \widetilde{Q}^{-1}G$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
12: **end for**
13: **return** $Q \leftarrow Q_{(:,[1:m,n+1:n+m])}$, $\Gamma' \leftarrow \Gamma$, $\Gamma \leftarrow \Gamma_{\mathrm{sav}}$, and $R = \begin{bmatrix} G_{(1:m,:)} \\ G_{(n+1:n+m,:)} \end{bmatrix}$.

and $Q^\top \Gamma Q = \Gamma'$, where

$$\begin{cases} \gamma'_\ell = \delta\gamma_\ell, & \delta = c^2 - s^2 = \pm 1, \\ \gamma'_j = \gamma_j, & j \neq \ell. \end{cases} \tag{3.18}$$

Remark 3.1. (i) Utilizing the special structure of $\boldsymbol{\Pi}^{-}$-matrix $G \in \boldsymbol{\Pi}^{-}_{2n\times 2m}$, $\widetilde{Q}^{-1}$ at lines 4, 7 and 10 of Algorithm 3.1 eliminates the $(n+\ell+1 : 2n, \ell)$ and $(\ell+1 : n, \ell)$ or the $(n+\ell, \ell)$th and $(\ell, n+\ell)$th or the $(\ell+1 : n, \ell)$ and $(n+\ell+1 : 2n, \ell)$ entries of G simultaneously, for $\ell = 1, \ldots, m$. (ii) Upon exit, Algorithm 3.1 computes $G = QR$, where $Q \in \mathbb{O}^{\boldsymbol{\Gamma}}_{2n}$ is a Γ-orthogonal matrix with respect to Γ and $R \in \mathbb{U}^{-}_{2n\times 2m}$. It is worth noting that Γ' is unknown before $G = QR$ is computed but it is unique, according to Theorem 3.1(i).

In the following, we use a small example with $n = 3$ and $m = 2$ by Wilkinson's diagram to illustrate the elimination process in computing a ΓQR factorization of G.

$$
\left[\begin{array}{cc|cc} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \hline \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{array}\right]
\xrightarrow[=\widetilde{Q}_1^{-1}]{Q_h(4:6;\boldsymbol{u})}
\left[\begin{array}{cc|cc} \times & \times & \times & \times \\ \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \hline \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{array}\right]
\xrightarrow[=\widetilde{Q}_2^{-1}]{Q_g(1;\alpha,\beta)}
\left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \times & \times & 0 & \times \\ \hline 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{array}\right]
$$

$$
\xrightarrow[=\widetilde{Q}_3^{-1}]{Q_h(1:3;\boldsymbol{u})}
\left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & \times \\ \hline 0 & \times & \times & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & \times \end{array}\right]
\xrightarrow[=\widetilde{Q}_4^{-1}]{Q_h(5:6;\boldsymbol{u})}
\left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & \times & 0 & \times \\ 0 & 0 & 0 & \times \end{array}\right]
$$

$$
\xrightarrow[=\widetilde{Q}_5^{-1}]{Q_g(2;\alpha,\beta)}
\left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ 0 & \times & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & \times \end{array}\right]
\xrightarrow[=\widetilde{Q}_6^{-1}]{Q_h(2:3;\boldsymbol{u})}
\left[\begin{array}{cc|cc} \times & \times & 0 & \times \\ 0 & \times & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline 0 & \times & \times & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & 0 \end{array}\right]
$$

In general,after m steps we have computed $3m$ $\mathit{\Gamma}$-orthogonal matrices $\widetilde{Q}_1^{-1}, \ldots, \widetilde{Q}_{3m}^{-1}$ such that $(\widehat{Q}_{3m}^{-1}, \ldots, \widehat{Q}_1^{-1})G = R$ is a $\boldsymbol{\mathit{\Pi}}^{-}$-upper triangular.

what does $(\widehat{Q}_{3m}^{-1}, \ldots, \widehat{Q}_1^{-1})$ mean?

Remark 3.2. Theorem 3.1(ii) reveals that almost all matrices in $\boldsymbol{\mathit{\Pi}}^{-}_{2n\times 2m}(m \leq n)$ have ΓQR factorizations. In practice, for a given $2n \times 2m$ $\boldsymbol{\mathit{\Pi}}^{-}$-matrix G, one way to construct its ΓQR factorization with respect to given $\mathit{\Gamma} \in \Gamma_{2n}$ is through reducing G to a $2n \times 2m$ $\boldsymbol{\mathit{\Pi}}^{-}$-upper triangular matrix by a sequence of $\mathit{\Gamma}$-orthogonal transformations: Hyp_Householder $\mathit{\Gamma}$-orthogonal transformations and Hyp_Givens $\mathit{\Gamma}$-orthogonal transformations. The Hyp_Householder transformation in (3.12a) may not exist if $\hat{\boldsymbol{a}}^{\mathrm{T}} J \hat{\boldsymbol{a}} = 0$. Similarly, the Hyp_Givens transformation in (3.17) may not exist if $|\alpha| = |\beta|$. In [1], it is said that these cases can occur when the matrix is artificially designed. There is clearly a numerical stability issue if $\hat{\boldsymbol{a}}^{\mathrm{T}} J \hat{\boldsymbol{a}} \approx 0$ or $|\alpha| \approx |\beta|$. The danger of severe cancellation can occurs and is discussed in [4, 5]. If a dangerous cancellation occurs at some ℓth step of Algorithm 3.1, it is recommended pre-multiply the current G by a randomly generated $\mathit{\Gamma}$-orthogonal $\widetilde{Q}^{-1}$ with $\widetilde{Q}^{\mathrm{T}} \mathit{\Gamma} \widetilde{Q}^{\mathrm{T}} = \mathit{\Gamma}'$. Then we set $G \leftarrow \widetilde{Q}^{-1} G$, $\mathit{\Gamma} \leftarrow \mathit{\Gamma}'$, and continue performing Algorithm 3.1 from the ℓth step. It usually can successfully circumvent the cancellation by this [4, 5].

4 Implicit Γ-orthogonality Theorem

Here and hereafter we suppose that $\mathscr{H} \in \boldsymbol{\Pi}_{2n}^{-}$ is $\boldsymbol{\Pi}^{-}$-symmetric with respect to $\Gamma \in \boldsymbol{\Gamma}_{2n}$.

Definition 4.1. Given $\boldsymbol{q}_1 \in \mathbb{R}^{2n}$ with $\boldsymbol{q}_1^\top \Gamma \boldsymbol{q}_1 = \pm 1$. For $1 \le m \le n$, the mth order *$\boldsymbol{\Pi}^{+}$-Krylov matrix of $\mathscr{H}$* on $\boldsymbol{q}_1$ is defined as

$$\begin{aligned} K_{2m} &\equiv K_{2m}(\mathscr{H}, \boldsymbol{q}_1) \\ &:= \left[\boldsymbol{q}_1, \mathscr{H}\boldsymbol{q}_1, \cdots, \mathscr{H}^{m-1}\boldsymbol{q}_1 \,|\, \Pi\boldsymbol{q}_1, \Pi(\mathscr{H}\boldsymbol{q}_1), \cdots, \Pi(\mathscr{H}^{m-1}\boldsymbol{q}_1)\right] \in \mathbb{R}^{2n\times 2m}. \end{aligned} \tag{4.1}$$

Let $\mathcal{K}_{2m} \equiv \mathcal{K}_{2m}(\mathscr{H}, \boldsymbol{q}_1)$ be the subspace spanned by the columns of K_{2m}.

Theorem 4.1. *Let $K_{2m} \equiv K_{2m}(\mathscr{H}, \boldsymbol{q}_1)$ be the $\boldsymbol{\Pi}^{+}$-Krylov matrix (4.1), where $m \le n$. Suppose* $\operatorname{rank}(K_{2m}) = 2m$, *and let $K_{2m} = Q_{2m}R_{2m}$ (with $Q_{2m} \in \mathbb{O}^{\boldsymbol{\Gamma}}_{2n\times 2m}$ and $R_{2m} \in \mathbb{U}^{-}_{2m}$) be a* ΓQR *factorization with respect to Γ and set $\Gamma' = Q_{2m}^\top \Gamma Q_{2m} \in \boldsymbol{\Gamma}_{2m}$. Then*

$$\mathscr{H} Q_{2m} = Q_{2m}T_{2m} + \boldsymbol{z}_m\boldsymbol{e}_m^\top - \Pi\boldsymbol{z}_m\boldsymbol{e}_{2m}^\top, \tag{4.2a}$$

$$Q_{2m}^\top \Gamma \boldsymbol{z}_m = Q_{2m}^\top \Gamma(\Pi\boldsymbol{z}_m) = 0, \tag{4.2b}$$

$$T_{2m} = (\Gamma' Q_{2m}^\top \Gamma)\mathscr{H} Q_{2m}, \tag{4.2c}$$

for some $\boldsymbol{z}_m \in \mathbb{R}^{2n}$, and $\Gamma' T_{2m}$ is unreduced $\boldsymbol{\Pi}^{+}$-sym-tridiagonal, i.e., T_{2m} is unreduced $\boldsymbol{\Pi}^{-}$-sym-tridiagonal with respect to Γ'.

Proof. Since $K_{2m} = Q_{2m}R_{2m}$ has full column rank and is the $2n \times 2m$ $\boldsymbol{\Pi}^{+}$-Krylov matrix by assumption, R_{2m} is $\boldsymbol{\Pi}^{+}$-upper triangular and nonsingular and so is R_{2m}^{-1}. Using $\mathscr{H}\Pi = -\Pi\mathscr{H}$, we have

$$\begin{aligned} \mathscr{H} K_{2m} &= \mathscr{H}\left[\boldsymbol{q}_1, \mathscr{H}\boldsymbol{q}_1, \cdots, \mathscr{H}^{m-1}\boldsymbol{q}_1, \Pi\boldsymbol{q}_1, \Pi(\mathscr{H}\boldsymbol{q}_1), \cdots, \Pi(\mathscr{H}^{m-1}\boldsymbol{q}_1)\right] \\ &= K_{2m}C_{2m} + \mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_m^\top - \Pi(\mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_{2m}^\top), \end{aligned} \tag{4.3}$$

where $C_{2m} = \operatorname{diag}(C_1, -C_1)$ with $C_1 = \begin{bmatrix} \boldsymbol{0}_{m-1}^\top & 0 \\ I_{m-1} & \boldsymbol{0}_{m-1} \end{bmatrix}$. Substituting K_{2m} by $Q_{2m}R_{2m}$ into (4.3), we get

$$\begin{aligned} \mathscr{H} Q_{2m} = Q_{2m}\Big[&\underbrace{R_{2m}C_{2m}R_{2m}^{-1} + \Gamma' Q_{2m}^\top \Gamma(\mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_m^\top - \Pi\mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_{2m}^\top)R_{2m}^{-1}}_{=:T_{2m}}\Big] \\ &+ (I - Q_{2m}\Gamma' Q_{2m}^\top \Gamma)(\mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_m^\top - \Pi\mathscr{H}^m\boldsymbol{q}_1\boldsymbol{e}_{2m}^\top)R_{2m}^{-1}. \end{aligned} \tag{4.4}$$

Set $\gamma_{mm} = \boldsymbol{e}_m^\top R_{2m}^{-1}\boldsymbol{e}_m = \boldsymbol{e}_{2m}^\top R_{2m}^{-1}\boldsymbol{e}_{2m}$ and $\boldsymbol{z}_m = \gamma_{mm}(I - Q_{2m}\Gamma' Q_{2m}^\top \Gamma)\mathscr{H}^m\boldsymbol{q}_1$. From (4.4), we have

$$\mathscr{H} Q_{2m} = Q_{2m}T_{2m} + \boldsymbol{z}_m\boldsymbol{e}_m^\top - \Pi\boldsymbol{z}_m\boldsymbol{e}_{2m}^\top. \tag{4.5}$$

From the fact that $Q_{2m}^\top \Gamma Q_{2m} = \Gamma'$ it follows that

$$Q_{2m}^\top \Gamma \boldsymbol{z}_m = Q_{2m}^\top \Gamma (\Pi \boldsymbol{z}_m) = 0. \tag{4.6}$$

Therefore $(\Gamma' Q_{2m}^\top \Gamma)\mathscr{H} Q_{2m} = T_{2m}$ by (4.5) and (4.6). Because C_{2m} in (4.4) is unreduced $\boldsymbol{\Pi}^-$-upper Hessenberg, by Proposition 2.1 we know that T_{2m} is unreduced $\boldsymbol{\Pi}^+$-upper Hessenberg. Furthermore, since $\mathscr{H}$ is $\boldsymbol{\Pi}^-$-symmetric with respect to Γ, $Q_{2m}^\top \Gamma \mathscr{H} Q_{2m}$ is $\boldsymbol{\Pi}^+$-sym-tridiagonal and thus T_{2m} is $\boldsymbol{\Pi}^-$-sym-tridiagonal with respect to Γ'. This completes the proof. □

Theorem 4.2. *Let $Q_{2m} \in \mathbb{R}^{2n\times 2m}$ $(m \le n)$ be a Γ-orthogonal with respect to Γ such that $Q_{2m}\boldsymbol{e}_1 = \boldsymbol{q}_1$. Let $\Gamma' = Q_{2m}^\top \Gamma Q_{2m}$. If Q_{2m} satisfies* (4.2a) *for some unreduced $\boldsymbol{\Pi}^+$-sym-tridiagonal, $\Gamma' T_{2m}$ and $\boldsymbol{z}_m \in \mathbb{R}^{2n}$, then*

$$\begin{aligned} K_{2m}(\mathscr{H}, \boldsymbol{q}_1) &= Q_{2m}\Big[\boldsymbol{e}_1, T_{2m}\boldsymbol{e}_1, \cdots, T_{2m}^{m-1}\boldsymbol{e}_1, \Pi\boldsymbol{e}_1, \Pi(T_{2m}\boldsymbol{e}_1), \cdots, \Pi(T_{2m}^{m-1}\boldsymbol{e}_1)\Big] \\ &=: Q_{2m}R_{2m} \end{aligned} \tag{4.7}$$

is a ΓQR *factorization of $K_{2m}(\mathscr{H}, \boldsymbol{q}_1)$ and* $\operatorname{rank}(K_{2m}(\mathscr{H}, \boldsymbol{q}_1)) = 2m$.

Proof. It holds that

$$\mathscr{H}\boldsymbol{q}_1 = \mathscr{H} Q_{2m}\boldsymbol{e}_1 = (Q_{2m}T_{2m} + \boldsymbol{z}_m\boldsymbol{e}_m^\top - \Pi\boldsymbol{z}_m\boldsymbol{e}_{2m}^\top)\boldsymbol{e}_1 = Q_{2m}T_{2m}\boldsymbol{e}_1. \tag{4.8}$$

Assume that $\mathscr{H}^{i-1}\boldsymbol{q}_1 = \mathscr{H}^{i-1}Q_{2m}\boldsymbol{e}_1 = Q_{2m}T_{2m}^{i-1}\boldsymbol{e}_1$ holds for $i = 2, \cdots, m-1$. Then

$$\begin{aligned} \mathscr{H}^i\boldsymbol{q}_1 &= \mathscr{H} Q_{2m}T_{2m}^{i-1}\boldsymbol{e}_1 \\ &= (Q_{2m}T_{2m} + \boldsymbol{z}_m\boldsymbol{e}_m^\top - \Pi\boldsymbol{z}_m\boldsymbol{e}_{2m}^\top)T_{2m}^{i-1}\boldsymbol{e}_1 \\ &= Q_{2m}T_{2m}^i\boldsymbol{e}_1 + \boldsymbol{z}_m\boldsymbol{e}_m^\top T_{2m}^{i-1}\boldsymbol{e}_1 - \Pi\boldsymbol{z}_m\boldsymbol{e}_{2m}^\top T_{2m}^{i-1}\boldsymbol{e}_1. \end{aligned}$$

It can be verified that $\boldsymbol{e}_m^\top T_{2m}^{i-1}\boldsymbol{e}_1 = \boldsymbol{e}_{2m}^\top T_{2m}^{i-1}\boldsymbol{e}_1 = 0$. Therefore, we have $\mathscr{H}^i\boldsymbol{q}_1 = Q_{2m}T_{2m}^i\boldsymbol{e}_1$ and thus (4.7) holds. Furthermore, R_{2m} in (4.7) is nonsingular and $\boldsymbol{\Pi}^+$-upper triangular. Hence, $\operatorname{rank}(K_{2m}(\mathscr{H}, \boldsymbol{q}_1)) = 2m$. □

Theorem 4.3 (Implicit Γ-orthogonality theorem)**.** *Let $\mathscr{H} \in \boldsymbol{\Pi}_{2n}^-$ be $\boldsymbol{\Pi}^-$-symmetric with respect to Γ and $Q, \widetilde{Q} \in \mathbb{R}^{2n\times 2n}$ be two Γ-orthogonal $\boldsymbol{\Pi}^+$-matrices with respect to $\Gamma \in \boldsymbol{\Gamma}_{2n}$. Assume $Q\boldsymbol{e}_1 = \widetilde{Q}\boldsymbol{e}_1$ and let*

$$\Gamma' = Q^\top \Gamma Q, \quad \widetilde{\Gamma}' = \widetilde{Q}^\top \Gamma \widetilde{Q}.$$

If $\mathscr{H} Q = QT_{2n}$ and $\mathscr{H}\widetilde{Q} = \widetilde{Q}\widetilde{T}_{2n}$, where $\Gamma' T_{2n}$ and $\widetilde{\Gamma}'\widetilde{T}_{2n}$ are unreduced $\boldsymbol{\Pi}^+$-sym-tridiagonal, i.e., T_{2n} and $\widetilde{T}_{2n}$ are unreduced $\boldsymbol{\Pi}^-$-sym-tridiagonal with respect to Γ' and $\widetilde{\Gamma}'$, respectively, then $Q = \widetilde{Q}D$, $\Gamma' = \widetilde{\Gamma}'$, and $T_{2n} = D\widetilde{T}_{2n}D$ for some $D = \operatorname{diag}(J, J)$ with $J \in \mathbb{J}_n$.

Proof. By Theorem 4.2, it holds that

$$K_{2n}(\mathscr{H}, Q\boldsymbol{e}_1) = QR = \widetilde{Q}\widetilde{R} = K_{2n}(\mathscr{H}, \widetilde{Q}\boldsymbol{e}_1),$$

where R and $\widetilde{R}$ are nonsingular and $\boldsymbol{\Pi}^+$-upper triangular. From Theorem 3.1(i), we know that the ΓQR factorization of the nonsingular $K_{2n}(\mathscr{H}, Q\boldsymbol{e}_1)$ is unique modulo some $\boldsymbol{\Pi}^+$-diagonal $D = \operatorname{diag}(J, J)$ with $J \in \mathbb{J}_n$. Thus, $\widetilde{Q} = QD$, $\widetilde{R} = DR$, and consequently

$$\widetilde{\varGamma}' = \widetilde{Q}^\top \varGamma \widetilde{Q} = DQ^\top \varGamma QD = D\varGamma' D = \varGamma',$$
$$\widetilde{T}_{2n} = \widetilde{\varGamma}'\widetilde{Q}^\top \varGamma \mathscr{H} \widetilde{Q} = \varGamma' DQ^\top \varGamma \mathscr{H} QD = D(\varGamma' Q^\top \varGamma)\mathscr{H} QD = DT_{2n}D,$$

as expected. □

5 ΓQR **Algorithms**

Based on ΓQR factorizations of $\boldsymbol{\Pi}^-$-matrices and inspired by the usual QR algorithm for the standard eigenvalue problem [11], in this section, we will develop structure-preserving ΓQR algorithms for solving the LREP (1.4) of a $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$ with respect to $\varGamma \in \boldsymbol{\varGamma}_{2n}$. A straightforward extension of the usual QR algorithm is outlined in Algorithm 5.1.

Algorithm 5.1 The simple ΓQR algorithm

Input: $\mathscr{H} \in \boldsymbol{\Pi}_{2n}^-$ a $\boldsymbol{\Pi}^-$-symmetric matrix with respect to $\varGamma \in \boldsymbol{\varGamma}_{2n}$;
Output: $\varGamma' \mathscr{H} \in \mathrm{q}\mathbb{D}_{2n}^+$ ($\boldsymbol{\Pi}^+$-quasi-diagonal).

$\mathscr{H}_1 \leftarrow \mathscr{H}$, $\varGamma_1 \leftarrow \varGamma$, $i = 1$;
repeat
  compute the ΓQR factorization with respect to $\varGamma_i$: $\mathscr{H}_i = Q_i R_i$;
  $\varGamma_{i+1} \leftarrow Q_i^\top \varGamma_i Q_i \in \boldsymbol{\varGamma}_{2n}$, $\mathscr{H}_{i+1} \leftarrow R_i Q_i$;
  $i \leftarrow i + 1$;
until convergence $\mathscr{H} \leftarrow \mathscr{H}_i$.

Proposition 5.1. *The following statements holds for* Algorithm 5.1.

(i) $Q_i^{-1} = \varGamma_{i+1} Q_i^\top \varGamma_i$, $\mathscr{H}_{i+1} = Q_i^{-1} \mathscr{H}_i Q_i = R_i \mathscr{H}_i R_i^{-1}$, $\varGamma_{i+1}\mathscr{H}_{i+1} = Q_i^\top (\varGamma_i \mathscr{H}_i) Q_i$.

(ii) $\mathscr{H}_{i+1} = (Q_1 \cdots Q_i)^{-1} \mathscr{H} (Q_1 \cdots Q_i)$, $\varGamma_{i+1}\mathscr{H}_{i+1} = (Q_1 \cdots Q_i)^\top (\varGamma \mathscr{H})(Q_1 \cdots Q_i)$. *Furthermore,* $\mathscr{H}_i$ *is* $\boldsymbol{\Pi}^-$*-symmetric with respect to* $\varGamma_i$.

(iii) $\mathscr{H}_{i+1} = (R_i \cdots R_1) \mathscr{H} (R_i \cdots R_1)^{-1}$, $\varGamma_{i+1} = (Q_1 \cdots Q_i)^\top \varGamma (Q_1 \cdots Q_i)$.

(iv) $\mathscr{H}^i = (Q_1 \cdots Q_i)(R_i \cdots R_1)$.

Let the spectral decomposition of $\mathscr{H}$ be

$$\mathscr{H} X = X\Lambda \quad \text{with} \quad \Lambda \in \mathrm{q}\mathbb{D}_{2n}^-, \ X \in \boldsymbol{\Pi}_{2n}^+. \tag{5.1a}$$

For P as in (3.3), we have

$$P^\top \Lambda P = \operatorname{diag}(\Lambda_1, \cdots, \Lambda_\ell) \text{ with } \operatorname{eig}(\Lambda_i) = \{\pm\lambda_i\}, \text{ or } \operatorname{eig}(\Lambda_i) = \{\pm\lambda_i, \pm\bar{\lambda}_i\}. \tag{5.1b}$$

In light of the convergence proof of the HR algorithm in [7], we can also prove the convergence of Algorithm 5.1.

Theorem 5.1. *Given $\Gamma \in \boldsymbol{\Gamma}_{2n}$, let $\mathscr{H} \in \boldsymbol{\Pi}_{2n}^-$ be $\boldsymbol{\Pi}^-$-symmetric with respect to Γ having the spectral decomposition* (5.1). *Suppose $|\lambda_1| > \cdots > |\lambda_\ell| > 0$ and* Algorithm 5.1 *is executable for $\mathscr{H}$ in the sense that all* ΓQR *factorizations at* line 3 *exist. If the $\boldsymbol{\Pi}^+$-LU factorization of $X^{-1} = L_{\mathbf{x}} U_{\mathbf{x}}$ exists, where $L_{\mathbf{x}}^\top$, $U_{\mathbf{x}} \in \mathrm{q}\mathbb{U}_{2n}^+$ with $L_{\mathbf{x}}$ having 1×1 and/or 2×2 unit diagonal blocks, conforming to the block structure of Λ and if the* ΓQR *factorization of $X = Q_{\mathbf{x}} R_{\mathbf{x}}$ with respect to Γ exists, then $\mathscr{H}_i$ in* Algorithm 5.1 *converges to a $\boldsymbol{\Pi}^-$-quasi-diagonal matrix with its eigenvalues λ_i emerging in the order of $\lambda_1, \lambda_2, \ldots, \lambda_\ell$, as $i \to \infty$.*

Proof. From the assumption, it follows that $\Lambda^i L_{\mathbf{x}} \Lambda^{-i} = I + E_i$ with $E_i \to 0$ as $i \to \infty$. Let $(I + R_{\mathbf{x}} E_i R_{\mathbf{x}}^{-1}) = \widetilde{Q}_i \widetilde{R}_i$ be the ΓQR factorization with respect to $\Gamma' := Q_{\mathbf{x}}^\top \Gamma Q_{\mathbf{x}}$, and set $\widetilde{\Gamma}_{i+1} := \widetilde{Q}_i^\top \Gamma' \widetilde{Q}_i \in \boldsymbol{\Gamma}_{2n}$. It holds that $\widetilde{Q}_i \to I_{2n}$ because $E_i \to 0$.

For i sufficiently large, we have

$$\begin{aligned}
\mathscr{H}^i = X\Lambda^i X^{-1} &= X\Lambda^i L_{\mathbf{x}} \Lambda^{-i} \Lambda^i U_{\mathbf{x}} \\
&= X(I + E_i)\Lambda^i U_{\mathbf{x}} \\
&= Q_{\mathbf{x}}(I + R_{\mathbf{x}} E_i R_{\mathbf{x}}^{-1}) R_{\mathbf{x}} \Lambda^i U_{\mathbf{x}} \\
&= (Q_{\mathbf{x}} \widetilde{Q}_i) \widetilde{R}_i R_{\mathbf{x}} \Lambda^i U_{\mathbf{x}}
\end{aligned}$$

which gives a ΓQR factorization of $\mathscr{H}^i$. On the other hand, $\mathscr{H}^i = (Q_1 \cdots Q_i)(R_i \cdots R_1)$ by Proposition 5.1(ii). Now apply the uniqueness of the ΓQR factorization as stated in Theorem 3.1(i) to conclude that there is $D_i = \operatorname{diag}(J_i, J_i)$ with $J_i \in \mathbb{J}_n$ such that

$$(Q_{\mathbf{x}} \widetilde{Q}_i) D_i = Q_1 \cdots Q_i, \quad D_i(\widetilde{R}_i R_{\mathbf{x}} \Lambda^i U_{\mathbf{x}}) = R_i \cdots R_1,$$

and $\widetilde{\Gamma}_{i+1} = \Gamma_{i+1}$. By Proposition 5.1(ii), we have

$$\mathscr{H}_{i+1} = D_i \widetilde{Q}_i^{-1} Q_{\mathbf{x}}^{-1} \mathscr{H} Q_{\mathbf{x}} \widetilde{Q}_i D_i = D_i \widetilde{Q}_i^{-1} R_{\mathbf{x}} \Lambda R_{\mathbf{x}}^{-1} \widetilde{Q}_i D_i$$

which converges to a $\boldsymbol{\Pi}^-$-quasi-diagonal matrix with its eigenvalues emerging in the order of $\lambda_1, \lambda_2, \ldots, \lambda_\ell$, as $i \to \infty$. ◻

Algorithm 5.2 $\boldsymbol{\Pi}^-$-sym-tridiagonalization

Input: $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$ with respect to $\Gamma = \operatorname{diag}(J, -J)$ with $J = \operatorname{diag}(\gamma_1, \cdots, \gamma_n) \in \mathbb{J}_n$;

Output: $Q \in \mathbb{O}_{2n}^{\boldsymbol{\Gamma}}$ with respect to Γ, $\Gamma' = Q^\top \Gamma Q \in \boldsymbol{\Gamma}_{2n}$, and $\mathscr{H}' = Q^{-1}\mathscr{H}Q$ is a $\boldsymbol{\Pi}^-$-sym-tridiagonal matrix with respect to Γ'.

$Q \leftarrow I_{2n}$, $\Gamma_{\text{sav}} \leftarrow \Gamma$, $\mathscr{H}_{\text{sav}} \leftarrow \mathscr{H}$, $n' \leftarrow 2n$;
for $\ell = 1 : n-1$ **do**
  $\ell' \leftarrow n + \ell + 1$, $\boldsymbol{u} \leftarrow G_{(:,\ell)}$;
  compute Hyp_Householder Γ-orthogonal transformation $\widetilde{Q}^{-1} = (\mathcal{Q}_h)_{(\ell':n';\boldsymbol{u})}$ with respect to Γ (by (3.13));
  $Q \leftarrow Q\widetilde{Q}$, $\mathscr{H} \leftarrow \widetilde{Q}^{-1}\mathscr{H}\widetilde{Q}$, $\Gamma \leftarrow -\Gamma'$ (by (3.15));
  $\alpha \leftarrow \mathscr{H}_{(\ell+1,\ell)}$, $\beta \leftarrow \mathscr{H}_{(\ell',\ell)}$;
  compute Hyp_Givens Γ-orthogonal transformation $\widetilde{Q}^{-1} = (\mathcal{Q}_g)_{(\ell+1;\alpha,\beta)}$ with respect to Γ (by (3.17));
  $Q \leftarrow Q\widetilde{Q}$, $\mathscr{H} \leftarrow \widetilde{Q}^{-1}\mathscr{H}\widetilde{Q}$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
  $\boldsymbol{u} \leftarrow \mathscr{H}_{(:,\ell)}$;
  Compute Hyp_Householder Γ-orthogonal transformation $\widetilde{Q}^{-1} = (\mathcal{Q}_h)_{(\ell+1:n;\boldsymbol{u})}$ with respect to Γ (by (3.13));
  $Q \leftarrow Q\widetilde{Q}$, $\mathscr{H} \leftarrow \widetilde{Q}^{-1}\mathscr{H}\widetilde{Q}$, $\Gamma \leftarrow \Gamma'$ (by (3.18));
end for
return $\Gamma' \leftarrow \Gamma$, $\Gamma \leftarrow \Gamma_{\text{sav}}$, $\mathscr{H}' \leftarrow \mathscr{H}$, $\mathscr{H} \leftarrow \mathscr{H}_{\text{sav}}$;

Note that we set $(\mathcal{Q}_h)_{(\ell:m;\boldsymbol{u})} = I$ if $\ell = m$.

check red text

In what follows, using Algorithm 5.1 as the basis, we focus on developing an efficient structure-preserving ΓQR algorithm to solve the eigenvalue problem (1.4) for the $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$ with respect to a given Γ such as Γ_0 in (1.2). To do so, we first reduce $\mathscr{H}$ to its $\boldsymbol{\Pi}^-$-sym-tridiagonal form with respect to Γ and then use the two special Γ-orthogonal transformations described in section 3 to implicitly carry out lines 3 and 4 in Algorithm 5.1. The first phase, the $\boldsymbol{\Pi}^-$*-sym-tridiagonalization*, is given in Algorithm 5.2. To illustrate the elimination process in the $\boldsymbol{\Pi}^-$-sym-tridiagonalization, we trace actions on a small example with $n = 4$ in Table 5.1.

$$\mathscr{H} \leftarrow \left[\begin{array}{cccc|cccc} \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \hline \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \end{array}\right], \quad \begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_1^{-1}\mathscr{H}\widetilde{Q}_1 = \\ \widetilde{Q}_1^{-1} = \mathcal{Q}_h(6:8;\boldsymbol{u}) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & \times & \times & \times & \times & 0 & 0 \\ \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ \hline \times & \times & 0 & 0 & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \end{array}\right],$$

$$\begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_2^{-1}\mathscr{H}\widetilde{Q}_2 = \\ \widetilde{Q}_2^{-1} = \mathcal{Q}_g(2:\alpha;\beta) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times & \times \end{array}\right], \quad \begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_3^{-1}\mathscr{H}\widetilde{Q}_3 = \\ \widetilde{Q}_3^{-1} = \mathcal{Q}_h(2:4;\boldsymbol{u}) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & 0 & 0 & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & \times & \times & \times \\ 0 & \times & \times & \times & 0 & \times & \times & \times \\ 0 & \times & \times & \times & 0 & \times & \times & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & 0 & 0 \\ 0 & \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & 0 & \times & \times & \times \\ 0 & \times & \times & \times & 0 & \times & \times & \times \end{array}\right],$$

$$\begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_4^{-1}\mathscr{H}\widetilde{Q}_4 = \\ \widetilde{Q}_4^{-1} = \mathcal{Q}_h(7:8;\boldsymbol{u}) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & 0 & 0 & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & \times & \times & 0 \\ 0 & \times & \times & \times & 0 & \times & \times & \times \\ 0 & \times & \times & \times & 0 & 0 & \times & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & 0 & 0 \\ 0 & \times & \times & 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & 0 & \times & \times & \times \end{array}\right], \quad \begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_5^{-1}\mathscr{H}\widetilde{Q}_5 = \\ \widetilde{Q}_5^{-1} = \mathcal{Q}_g(3:\alpha;\beta) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & 0 & 0 & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & 0 & 0 & \times & \times \\ 0 & \times & \times & \times & 0 & 0 & \times & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & 0 & \times & \times & \times \end{array}\right],$$

$$\begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_6^{-1}\mathscr{H}\widetilde{Q}_6 = \\ \widetilde{Q}_6^{-1} = \mathcal{Q}_h(3:4;\boldsymbol{u}) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & 0 & 0 & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & 0 & 0 & \times & \times \\ 0 & 0 & \times & \times & 0 & 0 & \times & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & \times & \times & \times & 0 \\ 0 & 0 & \times & \times & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & 0 & 0 & \times & \times \end{array}\right], \quad \begin{array}{c} \mathscr{H} \leftarrow \widetilde{Q}_7^{-1}\mathscr{H}\widetilde{Q}_7 = \\ \widetilde{Q}_7^{-1} = \mathcal{Q}_g(4:\alpha;\beta) \end{array} \left[\begin{array}{cccc|cccc} \times & \times & 0 & 0 & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 & \times & 0 & 0 \\ 0 & \times & \times & \times & 0 & 0 & \times & 0 \\ 0 & 0 & \times & \times & 0 & 0 & 0 & \times \\ \hline \times & 0 & 0 & 0 & \times & \times & 0 & 0 \\ 0 & \times & 0 & 0 & \times & \times & \times & 0 \\ 0 & 0 & \times & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & 0 & 0 & \times & \times \end{array}\right].$$

Table 5.1: The $\boldsymbol{\Pi}^-$-sym-tridiagonalization for $n = 4$

In general, after $n-1$ step in $\boldsymbol{\Pi}^-$-sym-tridiagonalization, we have computed $3n-2$ Γ-orthogonal matrices $\widetilde{Q}_1, \cdots, \widetilde{Q}_{3n-2}$ such that

$$\big(\widetilde{Q}_1 \cdots \widetilde{Q}_{3n-2}\big)^{-1} \mathscr{H} \big(\widetilde{Q}_1 \cdots \widetilde{Q}_{3n-2}\big) = \mathscr{H}'$$

is $\boldsymbol{\Pi}^-$-sym-tridiagonal with respect to Γ'.

As in the usual QR algorithm, the shift technique should be incorporated to accelerate the convergence of the simple ΓQR algorithm – Algorithm 5.1. By Proposition 2.2, we choose the filtering polynomials $p(x)$ as

$$\begin{cases} p(x) = (x-\lambda)(x+\lambda) & \text{for real or imaginary } \lambda, \\ p(x) = (x-\lambda)(x+\lambda)(x-\bar{\lambda})(x+\bar{\lambda}) & \text{for complex } \lambda \end{cases} \tag{5.2}$$

to ensure $p(\mathscr{H}) \in \boldsymbol{\Pi}_{2n}^+$. On the other hand, from Theorem 4.3, because of the uniqueness of the $\boldsymbol{\Pi}^-$-sym-tridiagonalization of $\mathscr{H}$, the ΓQR factorization can be performed without explicitly computing the ΓQR factorization of $p(\mathscr{H})$. It only needs to construct a Γ-orthogonal transformation Q to reduce the first column of $p(\mathscr{H})$ to a vector parallel to $\boldsymbol{e}_1$. We outline the implicit multi-shift ΓQR algorithm in Algorithm 5.3.

Remark 5.1. (i) In Algorithm 5.3, lines 11–13 can be executed in two substeps with $p_1(x)$ and $p_2(x)$, respectively, where

$$p_1(x) = (x-\lambda_1)(x+\lambda_1), \quad p_2(x) = (x-\lambda_2)(x+\lambda_2)$$

for real or purely imaginary λ_1 and λ_2, and

$$p_1(x) = (x-\lambda_1)(x-\bar{\lambda}_1), \quad p_2(x) = (x+\lambda_1)(x+\bar{\lambda}_1)$$

for complex λ_1. Doing so enables that all computations are done in the real arithmetics.

(ii) There are many other structure-preserving approaches as discussed in Section 1. Based on the characteristic analysis of these algorithms, we will compare the performance of the ΓQR algorithm with that of the PQR algorithm [16] in our numerical studies. The flop counts of the implicit multi-shift ΓQR algorithm and the PQR algorithm for a $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$ with respect to Γ are summarized in Table 5.2. In each phase, the ΓQR algorithm consumes less than the PQR algorithm, especially in each iterative step in Phase ii. This is because the PQR algorithm cannot take advantage of the symmetric structures in JA, JB of (1.4b) but has to treat them like an n-by-n nonsymmetric matrix.

Algorithm 5.3 Implicit Multi-shift ΓQR Algorithm

Input: $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$ with respect to $\Gamma = \mathrm{diag}(J, -J)$ with $J = \mathrm{diag}(\gamma_1, \cdots, \gamma_n) \in \mathbb{J}_n$, and tolerance ϵ;

Output: $Q \in \mathbb{O}_{2n}^{\boldsymbol{\Gamma}}$ with respect to Γ, $\Gamma' = Q^\top \Gamma Q \in \boldsymbol{\Gamma}_{2n}$, $\Lambda = Q^{-1}\mathscr{H}Q \in \mathrm{q}\mathbb{D}_{2n}^-$;

$\Gamma_{\mathrm{sav}} \leftarrow \Gamma$, $\mathscr{H}_{\mathrm{sav}} \leftarrow \mathscr{H}$, $Q \leftarrow I_{2n}$, $\Lambda_i \leftarrow \emptyset$ $(i = 1, 2)$;
while $n > 2$ **do**
  Use Algorithm 5.2 to perform $\boldsymbol{\Pi}^-$-sym-tridiagonalization: $\mathscr{H} \leftarrow \widetilde{Q}^{-1}\mathscr{H}\widetilde{Q}$, $Q \leftarrow Q\widetilde{Q}$, $\Gamma \leftarrow \Gamma'$ (Γ' is an output of Algorithm 5.2);
  if $|\mathscr{H}_{(n,n-1)}| < \epsilon(|\mathscr{H}_{(n-1,n-1)}| + |\mathscr{H}_{(n,n)}|)$ **then**
    $\Lambda_1 \leftarrow \mathrm{diag}(\mathscr{H}_{(n,n)}, \Lambda_1)$, $\Lambda_2 \leftarrow \mathrm{diag}(\mathscr{H}_{(2n,n)}, \Lambda_2)$,
    $\mathbb{I} = [1, \cdots, n-1, n+1, \cdots, 2n-1]$, $\mathscr{H} \leftarrow \mathscr{H}_{(\mathbb{I},\mathbb{I})}$, $\Gamma \leftarrow \Gamma_{(\mathbb{I},\mathbb{I})}$, $n \leftarrow n-1$;
  else
    if $|\mathscr{H}_{(n-1,n-2)}| < \epsilon(|\mathscr{H}_{(n-2,n-2)}| + |\mathscr{H}_{(n-1,n-1)}|)$ **then**
      $\Lambda_1 \leftarrow \mathrm{diag}(\mathscr{H}_{([n-1,n],[n-1,n])}, \Lambda_1)$, $\Lambda_2 \leftarrow \mathrm{diag}(\mathscr{H}_{([2n-1,2n],[n-1,n])}, \Lambda_2)$,
      $\mathbb{I} = [1, \cdots, n-2, n+1, \cdots, 2n-2]$, $\mathscr{H} \leftarrow \mathscr{H}_{(\mathbb{I},\mathbb{I})}$, $\Gamma \leftarrow \Gamma_{(\mathbb{I},\mathbb{I})}$, $n \leftarrow n-2$;
    else
      $\mathbb{I} = [n-1, n, 2n-1, 2n]$, $H_4 = \mathscr{H}_{(\mathbb{I},\mathbb{I})}$, and compute $\mathrm{eig}(H_4) = \{\pm l_1, \pm l_2\}$;
      $\boldsymbol{h} = p(\mathscr{H})\boldsymbol{e}_1$, where $p(x)$ is as given in (5.2) (see also Remark 5.1(i)).
      construct the Γ-orthogonal transformation Q_1 such that $Q_1^{-1}\boldsymbol{h} = h\boldsymbol{e}_1$;
      $\mathscr{H} \leftarrow Q_1^{-1}\mathscr{H}Q_1,\ Q \leftarrow QQ_1,\ \Gamma \leftarrow \Gamma'$;
    end if
  end if
end while
$\Lambda := \begin{bmatrix} \Lambda_1 & \Lambda_2 \\ -\Lambda_2 & -\Lambda_1 \end{bmatrix} \in \mathrm{q}\mathbb{D}_{2n}^-$, $\Gamma' \leftarrow \Gamma$, $\Gamma \leftarrow \Gamma_{\mathrm{sav}}$, $\mathscr{H} \leftarrow \mathscr{H}_{\mathrm{sav}}$.

Methods	Phase		Flop
ΓQR	i	$\boldsymbol{\Pi}^-$-sym-tridiagonalization on $\mathscr{H}$ by Algorithm 5.2	$8n^3$
	ii	one step of implicit double-shift ΓQR iteration (Algorithm 5.3)	$120n$
PQR	i	Hessenberg-triangular reduction by Householder transformation on $JKJM$ in (1.5)	$11n^3$
	ii	one step of implicit double-shift PQR iteration [14]	$35n^2$

Table 5.2: The flop counts of the ΓQR algorithm and the PQR algorithm

6 Numerical Experiments

To test the efficiency of ΓQR algorithm, we borrow K and M in the numerical example of [2] for the sodium dimer Na_2 with order $n = 1862$. They are symmetric positive definite. We then recover the Casida's eigenvalue problem as in (1.1) by $A = \frac{1}{2}(K + M) - 4.88I_n$ and $B = \frac{1}{2}(K - M)$ with an excitation energy 4.88, and reset $K = A - B$, $M = A + B$. In Table 6.1, we list the CPU time by the ΓQR algorithm and PQR algorithm for the computation of eigenvalues of $\mathscr{H} = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}$ and KM, respectively.

All numerical computations are carried out by MATLAB Version 2014b, on a MacBook Pro with a 2.8GHz Intel Core i7 processor and 8GB RAM, with the unit machine roundoff $\mathfrak{u} = 2^{-53} = 1.11 \times 10^{-16}$.

Methods		Phase	Time (secs.)
ΓQR	i	$\boldsymbol{\Pi}^-$-sym-tridiagonalization of $\mathscr{H}$ with Q accumulated	326.05
	ii	Implicit ΓQR algorithm (Algorithm 5.3)	399.23
PQR[1]	i	Hessenberg-triangular reduction on KM	643.02
	ii	Implicit PQR algorithm	2078.09

Table 6.1: The CPU time by ΓQR and PQR.

Table 6.1 shows that the PQR algorithm takes about 3.6 times as much the CPU time as ΓQR algorithm does. The ΓQR algorithm is much cheaper than the PQR algorithm, as expected from Table 5.2.

To demonstrate accuracies in computed approximations, we calculate the relative errors of eigenvalues and the normalized residual norms for the jth approximate eigenpair $(\mu_j, \boldsymbol{z}_j)$:

change $e(\mu_j)$ to $\epsilon(\mu_j)$ in all figures

$$\epsilon(\mu_j) = \frac{|\mu_j - \lambda_j|}{|\lambda_j|} \quad \text{and} \quad r(\mu_j) = \frac{||\mathscr{H}\boldsymbol{z}_j - \mu_j \boldsymbol{z}_j||_1}{(\|\mathscr{H}\|_1 + |\mu_j|)||\boldsymbol{z}_j||_1},$$

where λ_j denotes the jth "exact" eigenvalue of $\mathscr{H}$ obtained by MATLAB's function `eig`.

The approximate eigenpair $(\mu_j, \boldsymbol{z}_j)$ is computed as follows: (1) apply the inverse iteration with the computed eigenvalue μ_j^0 (by Algorithm 5.3) as the shift to the $\boldsymbol{\Pi}^-$-sym-tridiagonal matrix (an output of Algorithm 5.2) to compute an approximate eigenpair $(\tilde{\mu}_j, \tilde{\boldsymbol{z}}_j)$ of the $\boldsymbol{\Pi}^-$-sym-tridiagonal matrix, and (2) apply the inverse iteration again on $(\tilde{\mu}_j, \widetilde{Q}\tilde{\boldsymbol{z}}_j)$ to the original $\boldsymbol{\Pi}^-$-symmetric $\mathscr{H}$ ($\widetilde{Q}$ is another output of Algorithm 5.2) to get the corresponding approximate eigenpair $(\mu_j, \boldsymbol{z}_j)$ of the original $\mathscr{H}$. On the other hand, the approximate eigenpair of the PQR algorithm is computed by applying the inverse

why does ΓQR compute eigenpairs in a different way from PQR?

[1]jupiter.math.nctu.edu.tw/∼wwlin/code/PQZ.zip

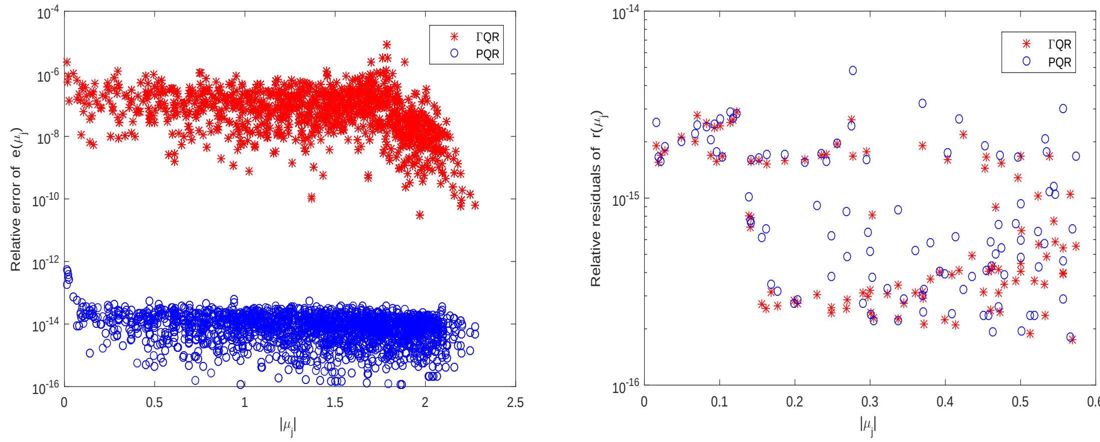

Figure 6.1: *Left:* relative errors of eigenvalues; *Right:* relative residual norm of eigenpairs.

iteration with the computed eigenvalue as the shift directly to the original $\boldsymbol{\Pi}^-$-symmetric matrix $\mathscr{H}$.

Therefore, the dominant step for the computation of eigenpairs by the ΓQR algorithm or the PQR algorithm is the LU factorization of the matrix $\mathscr{H} - \mu_j I$ for the inverse iteration. As before, the ΓQR algorithm is slightly more expensive than the PQR algorithm because an extra linear system of the $\boldsymbol{\Pi}^-$-sym-tridiagonal matrix needs to be solved with $O(n)$ flop counts.

In Figure 6.1 (left), we plot the relative errors of $\epsilon(\mu_j)$ for $j = 1, 2, \ldots, 1862$. Unfortunately, we see that the ΓQR algorithm achieves only half of the accuracy that the PQR algorithm can. This is because the Hyp_Householder and Hyp_Givens transformations are not orthogonal matrices which lead to loss of accuracy during the reduction/iteration process in the ΓQR algorithm. However, the Hyp_Householder and Hyp_Givens transformations are Γ-orthogonal, which are strongly structure-preserving for $\boldsymbol{\Pi}^-$-symmetric matrix with respect to Γ, and mutually contain so that the entry sizes of the reduced $\boldsymbol{\Pi}^-$-symmetric matrix always achieve a balanced state. This is the reason why the ΓQR algorithm still keep the half accuracy.

This reason is too vague.

In Figure 6.1 (right), we plot the normalized residual norms $r(\mu_j)$, $j = 1, \ldots, 100$ for the first 100 smallest positive eigenvalues of $\mathscr{H}$. It is clear that if all eigenpairs are obtained in this way, then the cost will dominant those of Algorithm 5.2 and 5.3. But computing different eigenpairs by the inverse iteration are highly independent and thus highly parallelizable.

7 Conclusions

In this paper, we have developed an efficient implicit multi-shift ΓQR algorithm for solving the linear response eigenvalue problem (LREP) in (1.1) structurally. This algorithm relies on two basic Γ-orthogonal transformations, which preserve $\boldsymbol{\Pi}^-$-symmetric structure of $\mathscr{H}$ with respect to Γ throughout the whole computation. Thus the computed eigenvalues and eigenvectors are guaranteed to appear pairwise as in $\{(\lambda,\boldsymbol{x}),(-\lambda,\Pi\boldsymbol{x})\}$ for a real or purely imaginary eigenvalue λ and in $\{(\lambda,\boldsymbol{x}),(-\lambda,\Pi\boldsymbol{x}),(\bar{\lambda},\bar{\boldsymbol{x}}),(-\bar{\lambda},\Pi\bar{\boldsymbol{x}})\}$ for a true complex eigenvalue λ. Note that, these structures will be lost if the Γ-orthogonality is not preserved owing to roundoff errors, as in the HR algorithm [7] and the usual QR algorithm. We accelerate the convergence of the ΓQR algorithm by using the double-shift technique based on the implicit Γ-orthogonality theorem, the final algorithm can be found in Algorithm 5.3. To compare with the block structure-preserving periodic QR algorithm, our algorithm costs much less than the PQR algorithm, and furthermore, the numerical experiment shows that the ΓQR algorithm can compute eigenpairs overall as accurate as the PQR algorithm. In summary, the ΓQR algorithm is an efficient structure-preserving algorithm for solving the $\boldsymbol{\Pi}^-$-symmetric eigenvalue problem compared with the other existing algorithms.

This contradicts Figure 6.1 (left). I suggest we drop the plots for relative errors because we don't know if the "exact eigenvalues" by **eig** are truly exact. PQR matches well with QR in computed eigenvalues because both are QR-based alg.

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