A New Real Structure-preserving Quaternion QR Algorithm

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Abstract

New real structure-preserving decompositions are introduced to develop fast and robust algorithms for the (right) eigenproblem of general quaternion matrices. Under the orthogonally $J_{RS}$-symplectic transformations, the Francis $J_{RS}$-QR step and the $J_{RS}$-QR algorithm are firstly proposed for $J_{RS}$-symmetric matrices and then applied to calculate the Schur forms of quaternion matrices. A novel quaternion Givens matrix is defined and utilized to compute the QR factorization of quaternion Hessenberg matrices. An implicit double shift quaternion QR algorithm is presented with a technique for automatically choosing shifts and within real operations. Numerical experiments are provided to demonstrate the efficiency and accuracy of newly proposed algorithms.

Key words. structured matrices; structure-preserving method; quaternion QR algorithm; quaternion eigenvalue problem.

1 Introduction

Quaternion matrices play an increasing important role in many fields of scientific research, both in theory and applications. The topics of quaternions are viewed of interest if the result is rather different than that of real and complex cases or the method is novel. The convenience of geometric representation and the stability of calculation make quaternions the favourite of scientists and engineers when they develop mathematical models to simulate and analysis physics phenomena.

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Quaternion was introduced to represent points in space by Sir William Rowan Hamilton on Monday 16 October 1843 in Dublin [12, 14]. During the remainder of his life, Hamilton tried hard to popularize quaternions by studying and teaching them. He founded a school of “quaternionists”, and wrote several books to promote quaternions. Elements of Quaternions [13] is his last and longest book. The team of promoting quaternions expanded quickly, not only including Hamilton and his students. Finkelstein et al [8, 9] built the foundations of quaternionic quantum mechanics; Dixon [6], Gürsey and Tze [11] renewed interest in algebrization and geometrization of physical theories by non-commutative fields; and many others. Primarily due to their utility in describing spatial rotations, quaternions have been widely used in and not limited in computer graphics [27], bioinformatics [26], control theory and physics since the late 20th century.

Recently, the book Topics in Quaternion Linear Algebra [23], written by Leiba Rodam, devotes entirely quaternionic linear algebra and matrix analysis, consisting of two parts. In the first part, fundamental properties and constructions of quaternionic linear algebra are explained, including matrix decompositions, numerical ranges, Jordan and Kronecker canonical forms, etc. In the second part, the canonical forms of quaternion pencils with symmetries and the exposition approaches that of a research monograph are emphasised. This book is an excellent reference source for working mathematicians in both theoretical and applied areas.

Because of noncommutative multiplication of quaternions, we have two different quaternionic eigenvalues: the left eigenvalue and the right eigenvalue. The right eigenvalue theory of quaternion matrices parallels that of complex eigenvalues of complex matrices in some sense, but the behavior of left eigenvalues is quite unexpected [33] and references therein. Most of practical quaternion models require to calculate the right eigenvalues and corresponding eigenvectors of quaternion matrices, while the investigation of left eigenvalues is mainly driven by purely mathematical interest. The distribution of the left and right eigenvalues of quaternion matrices has been well studied by mathematicians. For instance, Zhang [34] proposed the Geršgorin type theorems for right eigenvalues and left eigenvalues. On the contrast, there is still no systematic approach feasible for calculating the left eigenvalues of quaternion matrices with dimensions higher than three, and there is an extreme lack of fast and stable algorithms of computing the right eigenvalues of general quaternion matrices as well.

Non-commutativity of quaternions blocks lots of classic algorithms being directly used to solve quaternionic (right) eigenproblems. People have two choices of computing the right eigenvalues of general quaternion matrices: the quaternion QR algorithm [1] and the well-known real or complex counterpart method [16, 20, 33]. Bunse-Gerstner, Byers and Mehrmann [11] made a notable contribution on proposing the double-implicit-shift strategy and the Francis QR algorithm for quaternion matrices, and on calculating the quaternion Schur form with quaternion unitary similarity transformations. They also proposed the underlying theory of the quaternion QR algorithm, including the uniqueness and the preservation of the Hessenberg form, and indicated that such algorithm is backward stable. As the second choice, the real or complex counterpart method equivalently transforms the quaternionic right eigenproblem into the eigenproblem of a real (or complex) matrix with dimension expanded four (or two) times. Its efficiency is now challenged by the increasing dimensions of quaternion matrices from applied fields, because of expanding the necessary operation flops and storage space by several times. This new trouble is due to overlooking algebraic structures of the real (or complex) counterpart.

The real structure-preserving strategy is to develop fast and stable algorithms relying on
structures of the quaternion matrix and its real counterpart and only processing real operations. The aim is to combine the stability of quaternion operations and the rapidity of real calculations without dimension expanding. In essence, the real structure-preserving algorithms have comparable operation flops and storage space with the algorithms based on quaternion operations. The multiple symmetry structures of the real counterpart were introduced in [15] and had been applied into computing many decompositions of quaternion matrices. The real structure-preserving tridiagonalization algorithm in [15] reduced a Hermitian quaternion matrix into a real symmetric and tridiagonal matrix of the same order, with the eigen information preserved. A structure-preserving LU decomposition based on the structure-preserving Gauss transformation was proposed for quaternion matrices in [31]. Four kinds of quaternion Householder based transformations were compared with each other on their computation amounts and assignment numbers in the calculation of the QRD and SVD of quaternion matrices in [21]. These real structure-preserving algorithms have comparable stability and accuracy with the quaternion-operation-based algorithms. To the best of our knowledge, there are still no real structure-preserving algorithms of solving the right eigenvalue problem of non-Hermitian quaternion matrices, which is a very difficult and important problem in quaternionic linear algebra and its applications. We will propose a new real structure-preserving QR algorithm for general quaternion matrices, with costing about a quarter of arithmetic operations and storage space of applying the conventional QR algorithm on their real counterparts.

This paper is organized as follows. In Section 2 we present some properties of quaternion matrices and the real counterparts. In Section 3 we firstly propose the structure-preserving decompositions, including JRS-Hessenberg, QR and Schur decompositions, and then present the real structure-preserving $JRS$-Hessenberg QR iteration. In Section 4 we present a new fast quaternion Francis QR algorithm. In Section 5 we provide four numerical experiments. Finally in Section 6 we give several concluding remarks.

2 Preliminaries

In this section we present some basic results for quaternion matrices and their real counterparts. Let $\mathbb{H}$ denote the division ring generated by 1, $i$, $j$ and $k$, with identity 1 and

$$i^2 = j^2 = k^2 = ijk = -1.$$  

2.1 Quaternion matrices and $JRS$-symmetric matrices

A quaternion matrix $Q \in \mathbb{H}^{m \times n}$ is of the form

$$Q = Q_0 + Q_1 i + Q_2 j + Q_3 k, \quad Q_0, \ldots, Q_3 \in \mathbb{R}^{m \times n},$$

and its conjugate transpose is defined as $Q^* = Q_0^T - Q_1^T i - Q_2^T j - Q_3^T k$. A quaternion matrix $Q$ has right linearly independent columns (or in other words, $Q$ is full of column rank) if and only if $Qx = 0$ has a unique solution $x = 0$, and moreover, the columns of $Q$ are orthogonal to each other if $Q^* Q = I$. The real counterpart of a quaternion matrix $Q$ is defined in [15] as

$$\Upsilon_Q = \begin{bmatrix} Q_0 & Q_2 & Q_1 & Q_3 \\ -Q_2 & Q_0 & Q_3 & -Q_1 \\ -Q_1 & -Q_3 & Q_0 & Q_2 \\ -Q_3 & Q_1 & -Q_2 & Q_0 \end{bmatrix} \in \mathbb{R}^{4m \times 4n}. \quad (2.1)$$

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Many computational problems of quaternion matrices can be proceeded by corresponding real counterparts, with giving a rise of the dimension-expanding obstacle when the original quaternion matrix is huge. Such trouble can be solved if we sufficiently apply the structures of real counterparts in the processing of calculation. So we need to generalize the definitions of JRS-symmetric and symplectic (square) matrices in [15] into rectangular matrices.

**Definition 2.1.** Define three unitary matrices

\[ J_n = \begin{bmatrix} 0 & 0 & -I_n & 0 \\ 0 & 0 & 0 & -I_n \\ I_n & 0 & 0 & 0 \\ 0 & I_n & 0 & 0 \end{bmatrix}, R_n = \begin{bmatrix} 0 & -I_n & 0 & 0 \\ I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & I_n \\ 0 & 0 & -I_n & 0 \end{bmatrix}, S_n = \begin{bmatrix} 0 & 0 & 0 & -I_n \\ 0 & 0 & I_n & 0 \\ 0 & -I_n & 0 & 0 \\ I_n & 0 & 0 & 0 \end{bmatrix}. \]

(1) A real matrix \( M \in \mathbb{R}^{4m \times 4n} \) is called JRS-symmetric if \( J_m M J_n^T = M \), \( R_m M R_n^T = M \) and \( S_m M S_n^T = M \).

(2) If \( m \leq n \), a matrix \( O \in \mathbb{R}^{4m \times 4n} \) is called JRS-symplectic if \( O J_n O^T = J_m \), \( O R_n O^T = R_m \) and \( O S_n O^T = S_m \).

(3) A matrix \( W \in \mathbb{R}^{4n \times 4n} \) is called orthogonally JRS-symplectic if it is orthogonal and JRS-symplectic.

We can see that an \( n \)-by-\( n \) quaternion matrix \( Q \) is unitary if and only if its real counterpart \( \Upsilon_Q \) is orthogonal; and \( \Upsilon_Q \) is orthogonal if and only if it is orthogonally JRS-symplectic, because \( \Upsilon_Q \) is surely JRS-symmetric.

Notice that the set of JRS-symmetric matrices is closed under addition and multiplication.

**Lemma 2.1.** Suppose that \( M \in \mathbb{R}^{4m \times 4n} \), \( B \in \mathbb{R}^{4m \times 4\ell} \) and \( C \in \mathbb{R}^{4\ell \times 4n} \) are JRS-symmetric.

(1) \( M \) has a partitioning as

\[ M = \begin{bmatrix} M_0 & M_2 & M_1 & M_3 \\ -M_2 & M_0 & M_3 & -M_1 \\ -M_1 & -M_3 & M_0 & M_2 \\ -M_3 & M_1 & -M_2 & M_0 \end{bmatrix}. \]  \hspace{1cm} (2.2)

(2) For any \( \alpha, \beta \in \mathbb{R} \), \( \alpha M + \beta BC \) is JRS-symmetric.

(3) Moreover, if \( B \) and \( C \) are JRS-symplectic, then \( BC \) is also JRS-symplectic.

**Proof.** We only prove the item (3), because items (1) and (2) can be proved by direct calculation. Since \( B \) and \( C \) are JRS-symplectic, we have

\[ BJ_\ell B^T = J_m, \quad BR_\ell B^T = R_m, \quad BS_\ell B^T = S_m, \]

and

\[ CJ_\ell C^T = J_\ell, \quad CR_\ell C^T = R_\ell, \quad CS_\ell C^T = S_\ell. \]

Then

\[ (BC)J_n(BC)^T = B(CJ_n C^T)B^T = BJ_\ell B^T = J_m, \]
\[(BC)R_n(BC)^T = B(CR_nC^T)B^T = BR_tB^T = R_m,\]
\[(BC)S_n(BC)^T = B(CS_nC^T)B^T = BS_tB^T = S_m.\]

According to the second item in Definition 2.1, BC is JRS-symplectic.

With the real counterpart as a bridge, many properties of quaternion matrices can be obtained through studying JRS-symmetric matrices. This is based on an important discovery:

**Theorem 2.2.** A matrix \(M \in \mathbb{R}^{4m \times 4n}\) is JRS-symmetric if and only if \(M\) is a real counterpart of a quaternion matrix.

**Proof.** The theorem can be proved by straightforward computation.

The basic quaternion operations can be proceeded only by real arithmetic based on Lemma 2.1 and Theorem 2.2. For instance, suppose that \(Q, M, N \in H^{m \times n}, A, B \in H^{m \times \ell}, B \in H^{\ell \times n},\) and \(\alpha, \beta \in \mathbb{R},\) then

- \(Q = \alpha M + \beta N\) if and only if \(\Upsilon Q = \alpha \Upsilon M + \beta \Upsilon N\) \((14);\)
- \(Q = \alpha AB\) if and only if \(\Upsilon Q = \alpha \Upsilon A \Upsilon B\) \((15);\)
- \(\Upsilon Q^* = \alpha(\Upsilon Q)^T;\)
- \(\Upsilon Q^{-1} = (\Upsilon Q)^{-1}\) if \(Q\) is invertible;
- \(2\|Q\|_F = \|\Upsilon Q\|_F\) \((21),\) \(\|Q\|_2 = \|\Upsilon Q\|_2,\) and \(\rho(Q) = \rho(\Upsilon Q).\)

2.2 The quaternion eigenvalue problems

A pair \((x, \lambda)\) with nonzero vector \(x \in \mathbb{H}^n\) and \(\lambda \in \mathbb{H}\) is called the right (left) eigenpair of a quaternion matrix \(Q \in \mathbb{H}^{n \times n}\) if
\[Qx = x\lambda\ (Qx = \lambda x).\] (2.3)

The existence of right eigenvalues for any quaternion matrix was first proved by Berenner [3]. The left eigenvalue problem was raised by Cohn [5] and the existence of left eigenvalues for any quaternion matrix was proved by Wood [32] using a topological approach. Every \(n\)-by-\(n\) quaternion matrix has at least one left eigenvalue in \(\mathbb{H}\) [32], and however has exactly \(n\) right eigenvalues, which are complex numbers with nonnegative imaginary parts [3, 19]. Such right eigenvalues are called standard eigenvalues in [33]. Generally, left and right eigenvalues have no strong relation to each other. But they coincides when \(Q\) is a real matrix. Since the right eigenvalues have been well studied in theory and are more available in many applications, we only study the right eigenvalues of quaternion matrices and use “eigenvalue” to indicate the right eigenvalue for simplicity in the rest of this paper.

By adopting quaternion scalar products in \(\mathbb{H}^n\), we find states in one-to-one correspondence with unit rays of the form \(v = \{x\beta\}\), where \(x\) is a normalized vector and \(\beta\) is a quaternion phase of unity magnitude. The state vector, \(x\beta\), corresponding to the same physical state \(x\), is an eigenvector with eigenvalue \(\overline{\beta}\lambda\beta\), \(Q(x\beta) = (x\beta)(\overline{\beta}\lambda\beta)\). For real values of \(\lambda\), we find only one eigenvalue, otherwise we can find an infinite eigenvalue spectrum \([\lambda] = \{\lambda, \overline{\beta}_1\lambda\beta_1, \cdots, \overline{\beta}_\ell\lambda\beta_\ell, \cdots\}\) with \(\beta_\ell\) unitary quaternions, called the equivalence class containing \(\lambda\). The related set of eigenvectors \(\{x, x\beta_1, \cdots, x\beta_\ell, \cdots\}\) represents a ray. Any two
quaternions are similar if and only if their real parts and modules of imaginary parts are respectively equivalent \[33\] Theorem 2.2]. If \( \lambda \) is not real then \( |\lambda| \) contains only two complex numbers that are a conjugate pair. In fact, if \( \lambda = a + bi + cj + dk \) with \( c^2 + d^2 \neq 0 \) then we can choose \( \beta = a/|\alpha| \) with \( \alpha = b + \sqrt{b^2 + c^2 + d^2} - dj + ek \) such that \( \lambda_c = \overline{\lambda}\beta = a + \sqrt{b^2 + c^2 + d^2}i \in |\lambda| \). For this state the right eigenvalue equation in \((2.5)\) becomes

\[
Qv = v\lambda_c
\]

with \( v \in \mathbb{H}^n \) is a representative ray and \( \lambda_c \in \mathbb{C} \) is the corresponding standard eigenvalue. We will focus on computing the standard eigenvalues of quaternion matrices.

The following important results are recalled from \[23\] and \[33\]:

**Theorem 2.3** \((23, 33)\). Let \( Q \in \mathbb{H}^{n \times n} \). Then:

- (Schur’s triangularization theorem) there exists a unitary \( U \in \mathbb{H}^{n \times n} \) such that \( U^*QU \) is upper triangular with complex diagonal entries;
- if \( Q \) is Hermitian, then there exists a unitary \( U \in \mathbb{H}^{n \times n} \) such that \( U^*QU \) is diagonal and real;
- if \( Q \) is skew Hermitian, then there exists a unitary \( U \in \mathbb{H}^{n \times n} \) such that \( U^*QU \) is diagonal complex matrix with purely imaginary nonzero entries;
- if \( Q \) is unitary, then there exists a unitary \( U \in \mathbb{H}^{n \times n} \) such that \( U^*QU \) is diagonal and consists of unit complex numbers.

Define the quaternion Jordan block as

\[
J_m(\lambda) = \begin{bmatrix}
\lambda & 1 & 0 & \cdots & 0 \\
0 & \lambda & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\vdots & \vdots & \ddots & \ddots & \lambda \\
0 & 0 & \cdots & 0 & \lambda \\
\end{bmatrix} \in \mathbb{H}^{m \times m}.
\]

**Theorem 2.4** \((23, 33)\). Let \( Q \in \mathbb{H}^{n \times n} \). Then there exists an invertible \( X \in \mathbb{H}^{n \times n} \) such that

\[
X^{-1}QX = J_{m_1}(\lambda_1) \oplus \cdots \oplus J_{m_p}(\lambda_p), \lambda_1, \ldots, \lambda_p \in \mathbb{H}.
\]

The form \((2.5)\) is uniquely determined by \( Q \) up to arbitrary permutation of diagonal blocks and up to a replacement of \( \lambda_1, \ldots, \lambda_p \) with \( \lambda_1, \ldots, \lambda_p \) within the diagonal blocks where \( \lambda_s \in [\lambda_s], \ s = 1, \ldots, p \).

The (right) eigenvalues are continuous functions of the quaternion matrix.

**Theorem 2.5** \((23)\). Let \( Q \in \mathbb{H}^{n \times n} \) and let \( \lambda_1, \ldots, \lambda_s \) be all the distinct eigenvalues of \( Q \) in the closed upper complex half-plane \( \mathbb{C}_+ \). Then for every \( \epsilon > 0 \), there exists \( \delta > 0 \) such that if \( \Delta Q \in \mathbb{H}^{n \times n} \) satisfies \( \|\Delta Q\| < \delta \), then the eigenvalues of \( Q + \Delta Q \) are contained in the union

\[
\bigcup_{t=1}^s \{z \in \mathbb{C}_+ : |z - \lambda_t| < \epsilon\}.
\]
Recall that the eigenvalues in the closed upper complex half-plane \( \mathbb{C}_+ \) of a quaternion matrix is called standard eigenvalues.

For any two different \( n \)-dimensional quaternion vectors \( x, y \), if \( \|x\| = \|y\| \) and \( y^* x \in \mathbb{R} \), there exists a Householder matrix \( I - 2\omega \omega^* \) with \( \omega = (y - x)/\|y - x\| \) maps \( y \) to \( x \) \(^1\). Applying the Householder based transformations, we can calculate the QR factorization of quaternion matrix \( A \in \mathbb{H}^{n \times n} \), i.e., \( A = QR \), where \( Q \in \mathbb{H}^{n \times n} \) is unitary and \( R \in \mathbb{H}^{n \times n} \) is upper triangular \(^4\). As a milestone work, Bunse-Gerstner, Byers and Mehrmann in \(^1\) proposed the practical QR algorithm to calculate the Schur decomposition of a quaternion matrix. The bump chasing, double implicit shift method of the Francis QR iteration \(^{10, 28}\) were also carried over to the quaternion case with explicit algorithms listed in the appendix of \(^1\). The quaternion QR algorithm (\(^1\) Algorithm A5) is suitable for computing the Schur decomposition of a general quaternion matrix. Unfortunately quaternion arithmetic is quite expensive and to be avoided at all possible. We will show that there is a real equivalent of the Schur form and that the QR algorithm can be adapted to compute it in real arithmetic.

The way to combine the stability of quaternion operations and the rapidity of real calculations is to develop real structure-preserving algorithms based on the algebraic symmetry properties of the real counterpart. We find that the decompositions of quaternion matrices can be put into effect by the \( \text{JRS}\)-symmetry-preserving transformations of their real counterparts, and meanwhile, the accompanying dimension-expanding problem caused by the real counterpart method will vanish. This motivates us to develop the structure-preserving Hessenberg reduction and the real Schur form of \( \text{JRS}\)-symmetric matrices at first, and then design a new real structure-preserving Francis QR algorithm for quaternion matrices, which is expected to be fast and strongly backward stable. We emphasize that the real counterpart will not be generated in the newly proposed algorithms, and hence the operations will be directly applied on the real part and three imaginary parts of the quaternion matrix.

### 3 The structure-preserving methods

In this section, we propose the structure-preserving Hessenberg, QR and Schur decompositions of \( \text{JRS}\)-symmetric matrices and the real structure-preserving \( \text{JRS}\)-QR algorithm.

Firstly, we recall the fact that orthogonally \( \text{JRS}\)-symplectic equivalence transformations can preserve the \( \text{JRS}\)-symmetry \(^1\). From the second term of Definition 2.1 straightforward calculation indicates that every orthogonally \( \text{JRS}\)-symplectic matrix \( W \in \mathbb{R}^{4n \times 4n} \) has the block structure

\[
W = \begin{bmatrix}
W_0 & W_2 & W_1 & W_3 \\
-W_2 & W_0 & W_3 & -W_1 \\
-W_1 & -W_3 & W_0 & W_2 \\
-W_3 & W_1 & -W_2 & W_0
\end{bmatrix}, W_1, \cdots, W_3 \in \mathbb{R}^{n \times n}.
\]  

(3.1)

An example of orthogonally \( \text{JRS}\)-symplectic matrix is the generalized symplectic Givens rota-
A JRS-symmetric matrix $H \in \mathbb{R}^{4n \times 4n}$ is called an upper JRS-Hessenberg matrix if

$$
H = \begin{bmatrix}
H_0 & H_2 & H_1 & H_3 \\
-H_2 & H_0 & H_3 & -H_1 \\
-H_1 & -H_3 & H_0 & H_2 \\
-H_3 & H_1 & -H_2 & H_0
\end{bmatrix},
$$

(3.3)

where $H_0 \in \mathbb{R}^{n \times n}$ is an upper Hessenberg matrix, $H_1, H_2, H_3 \in \mathbb{R}^{n \times n}$ are upper triangular matrices. Moreover if all subdiagonal elements of $H_0$ are nonzeros, $H$ is called an unreduced upper JRS-Hessenberg matrix.

**Theorem 3.1.** Suppose that a JRS-symmetric matrix $M \in \mathbb{R}^{4n \times 4n}$ is of the form (2.2). Then there exists an orthogonally JRS-symplectic matrix $W \in \mathbb{R}^{4n \times 4n}$ such that $WMW^T = H$ is an upper JRS-Hessenberg matrix.
Proof. We prove the assertion by induction on the order \( n \). For \( n = 1 \), it is clear that the theorem is true. Suppose that for the case \( 1 \leq n < \ell \), there exists an orthogonally JRS-symplectic matrix \( W \in \mathbb{R}^{4n \times 4n} \) such that

\[
\tilde{W} M \tilde{W}^T = \begin{bmatrix}
\tilde{H}_0 & \tilde{H}_2 & \tilde{H}_1 & \tilde{H}_3 \\
-\tilde{H}_2 & \tilde{H}_0 & \tilde{H}_3 & -\tilde{H}_1 \\
-\tilde{H}_1 & -\tilde{H}_3 & \tilde{H}_0 & \tilde{H}_2 \\
-\tilde{H}_3 & \tilde{H}_1 & -\tilde{H}_2 & \tilde{H}_0
\end{bmatrix},
\]

(3.4)

where \( \tilde{H}_0 \in \mathbb{R}^{n \times n} \) is an upper Hessenberg matrix, \( \tilde{H}_{1,2,3} \in \mathbb{R}^{n \times n} \) are upper triangular matrices. For \( n = \ell \), denote

\[
M_0 = \begin{bmatrix}
m_{11}^{(0)} & m_{12}^{(0)} & m_{13}^{(0)} M_{14}^{(0)} \\
m_{21}^{(0)} & m_{22}^{(0)} & m_{23}^{(0)} M_{24}^{(0)} \\
m_{31}^{(0)} & m_{32}^{(0)} & m_{33}^{(0)} M_{34}^{(0)} \\
M_{41}^{(0)} & M_{42}^{(0)} & M_{43}^{(0)} M_{44}^{(0)}
\end{bmatrix}, \quad M_1 = \begin{bmatrix}
m_{11}^{(1)} & m_{12}^{(1)} & m_{13}^{(1)} M_{14}^{(1)} \\
m_{21}^{(1)} & m_{22}^{(1)} & m_{23}^{(1)} M_{24}^{(1)} \\
m_{31}^{(1)} & m_{32}^{(1)} & m_{33}^{(1)} M_{34}^{(1)} \\
M_{41}^{(1)} & M_{42}^{(1)} & M_{43}^{(1)} M_{44}^{(1)}
\end{bmatrix},
\]

\[
M_2 = \begin{bmatrix}
m_{11}^{(2)} & m_{12}^{(2)} & m_{13}^{(2)} M_{14}^{(2)} \\
m_{21}^{(2)} & m_{22}^{(2)} & m_{23}^{(2)} M_{24}^{(2)} \\
m_{31}^{(2)} & m_{32}^{(2)} & m_{33}^{(2)} M_{34}^{(2)} \\
M_{41}^{(2)} & M_{42}^{(2)} & M_{43}^{(2)} M_{44}^{(2)}
\end{bmatrix}, \quad M_3 = \begin{bmatrix}
m_{11}^{(3)} & m_{12}^{(3)} & m_{13}^{(3)} M_{14}^{(3)} \\
m_{21}^{(3)} & m_{22}^{(3)} & m_{23}^{(3)} M_{24}^{(3)} \\
m_{31}^{(3)} & m_{32}^{(3)} & m_{33}^{(3)} M_{34}^{(3)} \\
M_{41}^{(3)} & M_{42}^{(3)} & M_{43}^{(3)} M_{44}^{(3)}
\end{bmatrix},
\]

in which \( m_{st}^{(r)} \in \mathbb{R}, M_{s4}^{(r)} \in \mathbb{R}^{1 \times (\ell - 3)} \) and \( M_{4s}^{(r)} \in \mathbb{R}^{(\ell - 3) \times 1} \) and \( M_{44}^{(r)} \in \mathbb{R}^{(\ell - 3) \times (\ell - 3)}, r = 0, \ldots, 3, \ s, t = 1, 2, 3, \)

There are a series of generalized symplectic Givens rotations \( G_2, G_3, \ldots, G_\ell \in \mathbb{R}^{4n \times 4n} \) such that

\[
\tilde{M} := G_\ell \cdots G_3 G_2 M (G_\ell \cdots G_3 G_2)^T = \begin{bmatrix}
\tilde{M}_0 & \tilde{M}_2 & \tilde{M}_1 & \tilde{M}_3 \\
-\tilde{M}_2 & \tilde{M}_0 & \tilde{M}_3 & -\tilde{M}_1 \\
-\tilde{M}_1 & -\tilde{M}_3 & \tilde{M}_0 & \tilde{M}_2 \\
-\tilde{M}_3 & \tilde{M}_1 & -\tilde{M}_2 & \tilde{M}_0
\end{bmatrix},
\]

with

\[
\tilde{M}_0 = \begin{bmatrix}
m_{11}^{(0)} & \tilde{m}_{12}^{(0)} & \tilde{m}_{13}^{(0)} \tilde{M}_{14}^{(0)} \\
\gamma_{21} \tilde{m}_{22}^{(0)} & \tilde{m}_{23}^{(0)} & \tilde{m}_{24}^{(0)} \tilde{M}_{24}^{(0)} \\
\gamma_{31} \tilde{m}_{32}^{(0)} & \tilde{m}_{33}^{(0)} & \tilde{m}_{34}^{(0)} \tilde{M}_{34}^{(0)} \\
\Gamma_{41} \tilde{M}_{42}^{(0)} & \tilde{M}_{43}^{(0)} & \tilde{M}_{44}^{(0)}
\end{bmatrix}, \quad \tilde{M}_1 = \begin{bmatrix}
m_{11}^{(1)} & \tilde{m}_{12}^{(1)} & \tilde{m}_{13}^{(1)} \tilde{M}_{14}^{(1)} \\
0 & \tilde{m}_{22}^{(1)} & \tilde{m}_{24}^{(1)} \tilde{M}_{24}^{(1)} \\
0 & \tilde{m}_{32}^{(1)} & \tilde{m}_{34}^{(1)} \tilde{M}_{34}^{(1)} \\
0 & \tilde{M}_{42}^{(1)} & \tilde{M}_{44}^{(1)}
\end{bmatrix},
\]

\[
\tilde{M}_2 = \begin{bmatrix}
m_{11}^{(2)} & \tilde{m}_{12}^{(2)} & \tilde{m}_{13}^{(2)} \tilde{M}_{14}^{(2)} \\
0 & \tilde{m}_{22}^{(2)} & \tilde{m}_{24}^{(2)} \tilde{M}_{24}^{(2)} \\
0 & \tilde{m}_{32}^{(2)} & \tilde{m}_{34}^{(2)} \tilde{M}_{34}^{(2)} \\
0 & \tilde{M}_{42}^{(2)} & \tilde{M}_{44}^{(2)}
\end{bmatrix}, \quad \tilde{M}_3 = \begin{bmatrix}
m_{11}^{(3)} & \tilde{m}_{12}^{(3)} & \tilde{m}_{13}^{(3)} \tilde{M}_{14}^{(3)} \\
0 & \tilde{m}_{22}^{(3)} & \tilde{m}_{24}^{(3)} \tilde{M}_{24}^{(3)} \\
0 & \tilde{m}_{32}^{(3)} & \tilde{m}_{34}^{(3)} \tilde{M}_{34}^{(3)} \\
0 & \tilde{M}_{42}^{(3)} & \tilde{M}_{44}^{(3)}
\end{bmatrix},
\]

where \( \Gamma_{41} = [\gamma_{41}, \ldots, \gamma_{4\ell}] \), \( \gamma_{s1} = \sqrt{(m_{s1}^{(0)})^2 + (m_{s1}^{(1)})^2 + (m_{s1}^{(2)})^2 + (m_{s1}^{(3)})^2} \) \( (s = 2, 3, \ldots, \ell) \). Then we can generate a Householder matrix \( \mathcal{H}_2 \in \mathbb{R}^{\ell \times \ell} \) such that

\[
\mathcal{H}_2 \tilde{M}_0(:, 1) = [m_{11}^{(0)}, \tilde{\gamma}_{21}, 0, \ldots, 0]^T,
\]

and process the orthogonally JRS-symplectic transformation

\[
\hat{M} = [\mathcal{H}_2 \oplus \mathcal{H}_2 \oplus \mathcal{H}_2 \oplus \mathcal{H}_2] \tilde{M} \mathcal{H}_2 \oplus \mathcal{H}_2 \oplus \mathcal{H}_2 \oplus \mathcal{H}_2]^T = \begin{bmatrix}
\hat{M}_0 & \hat{M}_2 & \hat{M}_1 & \hat{M}_3 \\
-\hat{M}_2 & \hat{M}_0 & \hat{M}_3 & -\hat{M}_1 \\
-\hat{M}_1 & -\hat{M}_3 & \hat{M}_0 & \hat{M}_2 \\
-\hat{M}_3 & \hat{M}_1 & -\hat{M}_2 & \hat{M}_0
\end{bmatrix},
\]

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where \( \tilde{M}_s = H_2 \tilde{M}_s H_2^T, s = 0, \ldots, 3 \). Note that the submatrix of \( \tilde{M} \) by deleting the 1, \( \ell + 1, 2\ell + 1, 3\ell + 1 \) rows and columns is a \( 4(\ell - 1) \times 4(\ell - 1) \) \( JRS \)-symmetric matrix. By the introduction assumption, the theorem can be proved. \( \square \)

**Corollary 3.2.** Suppose that \( M \in \mathbb{R}^{4n \times 4n} \) is a \( JRS \)-symmetric matrix.

1. If \( M \) is also symmetric, there exists an orthogonally \( JRS \)-symplectic matrix \( W \in \mathbb{R}^{4n \times 4n} \) such that
   \[
   WMW^T = H_0 \oplus H_0 \oplus H_0 \oplus H_0, \tag{3.5}
   \]
   where \( H_0 \in \mathbb{R}^{n \times n} \) is a symmetric tridiagonal matrix \cite{15}.

2. If \( M \) is also skew-symmetric, there exists an orthogonally \( JRS \)-symplectic matrix \( W \in \mathbb{R}^{4n \times 4n} \) such that
   \[
   WMW^T = H \]
   has the form \( \tag{3.3} \)
   \[
   \text{with } H_0 = -H_0^T \in \mathbb{R}^{n \times n} \text{ tridiagonal and } H_1, H_2, H_3 \in \mathbb{R}^{n \times n} \text{ diagonal.}
   \]

### 3.2 The \( JRS \)-QR decomposition

In analogous processing, we define and calculate the \( JRS \)-QR decomposition of \( JRS \)-symmetric matrices.

**Definition 3.2.** A \( JRS \)-symmetric matrix \( R \in \mathbb{R}^{4m \times 4n} \) is called an upper \( JRS \)-triangular matrix if

\[
\begin{bmatrix}
R_0 & R_2 & R_1 & R_3 \\
-R_2 & R_0 & R_3 & -R_1 \\
-R_1 & -R_3 & R_0 & R_2 \\
-R_3 & R_1 & -R_2 & R_0
\end{bmatrix},
\]

where \( R_0 \in \mathbb{R}^{m \times n} \) is upper triangular, \( R_1, R_2, \) and \( R_3 \in \mathbb{R}^{m \times n} \) are strictly upper triangular. Moreover, if \( R_0 \) is also strictly upper triangular then \( R \) is called a strictly upper \( JRS \)-triangular matrix.

**Theorem 3.3.** Suppose that \( M \in \mathbb{R}^{4m \times 4n} \) is a \( JRS \)-symmetric matrix. Then there exists an orthogonally \( JRS \)-symplectic matrix \( W \in \mathbb{R}^{4m \times 4m} \) such that

\[
W^T \Upsilon_Q = R \in \mathbb{R}^{4m \times 4n}
\]

is an upper \( JRS \)-triangular form.

**Proof.** The theorem can be proved in a similar way with Theorem 3.1. \( \square \)

Notice that if \( n = 1 \), \( W \) acts like a Householder transformation to simultaneously delete nonzero elements of \( M \) besides \((1, 1), (m + 1, 2), (2m + 1, 3), (3m + 1, 4)\) positions; in this case we denote

\[
W = \text{house}(M). \tag{3.7}
\]

This notation will be used in the outlines of our algorithms.
3.3 The real JRS-Schur decomposition

The real JRS-Schur form can be introduced for JRS-symmetric matrices.

**Definition 3.3.** A JRS-symmetric matrix $T \in \mathbb{R}^{4n \times 4n}$ is called the real JRS-Schur form if

$$T = \begin{bmatrix}
T_0 & T_2 & T_1 & T_3 \\
-T_2 & T_0 & T_3 & -T_1 \\
-T_1 & -T_3 & T_0 & T_2 \\
-T_3 & T_1 & -T_2 & T_0
\end{bmatrix},$$

where $T_0 \in \mathbb{R}^{n \times n}$ is a real Schur form, $T_1$, $T_2$, and $T_3 \in \mathbb{R}^{n \times n}$ are upper triangular.

**Theorem 3.4.** Suppose that $M \in \mathbb{R}^{4n \times 4n}$ is a JRS-symmetric matrix. Then there exists an orthogonally JRS-symplectic matrix $W \in \mathbb{R}^{4n \times 4n}$ such that $W^T MW = T \in \mathbb{R}^{4n \times 4n}$ is a real JRS-Schur form.

Proof. The theorem can be proved in a similar way with Theorem 3.1. \qed

3.4 The structure-preserving JRS-Hessenberg QR iteration

Based on the previous structure-preserving decompositions, we turn to designing a real structure-preserving algorithm of computing the real JRS-Schur decomposition. Let $M \in \mathbb{H}^{4n \times 4n}$ be JRS-symmetric, then a practical JRS-QR algorithm can be written as

$$H = VMV^T$$
for $s = 1, 2, \ldots$

$$H = WR \text{ (JRS-QR decomposition)}$$
$$H = RW$$
end

where each $V, W \in \mathbb{R}^{4n \times 4n}$ is orthogonally JRS-symplectic and $R \in \mathbb{R}^{4n \times 4n}$ is upper JRS-triangular. When $M$ has complex eigenvalue this real iteration is associated with a difficulty that $H$ can never converge to JRS-triangular form. The expectations must be lowered and we must be content with the calculation of an alternative decomposition—the real JRS-Schur decomposition. If $V$ is chosen so that $H$ is upper JRS-Hessenberg, then the amount of work per iteration is reduced from $O(n^3)$ to $O(n^2)$.

The traditional QR algorithm can be adapted to compute a real JRS-Schur form of $M$ in real arithmetic.

$$H = VMV^T \text{ (JRS-Hessenberg reduction)}$$
for $s = 1, 2, \ldots$

Determine a scalar $\kappa$.

$$H - \kappa I = WR \text{ (JRS-QR decomposition)}$$
$$H = RW + \kappa I.$$ end

The reduction of $M$ to JRS-Hessenberg form is done in real arithmetic. If the Wilkinson shift $\kappa$ is real, the JRS-QR step results in a real matrix $H$. If $\kappa$ is complex, we simultaneously apply two JRS-QR steps, one with shift $\kappa$ and the other with shift $\overline{\kappa}$ to yield a matrix $\tilde{H}$. If

$$\tilde{W} \tilde{R} = (H - \kappa I)(H - \overline{\kappa} I)$$
is the JRS-QR decomposition of \((H - \kappa I)(H - \pi I)\), then

\[
\tilde{H} = \tilde{W}^T H \tilde{W}.
\]

Since

\[
(H - \kappa I)(H - \pi I) = H^2 - 2\text{Re}(\kappa)H + |\kappa|^2 I
\]
is real, so are \(\tilde{W}\) and \(\tilde{H}\). The strategy of working with complex conjugate Wilkinson shifts is so called the Francis double shift strategy. The complex arithmetic can be avoided by forming the matrix \(H^2 - 2\text{Re}(\kappa)H + |\kappa|^2 I\), computing its Q-factor \(\tilde{W}\), and then computing \(\tilde{H} = \tilde{W}^T H \tilde{W}\). Unfortunately, the formation of \(H^2 - 2\text{Re}(\kappa)H + |\kappa|^2 I\) requires \(O(n^3)\) operations. So we have to use a remarkable property of JRS-Hessenberg matrices to sidestep the formation of \(H^2 - 2\text{Re}(\kappa)H + |\kappa|^2 I\). Before turning to this property, we first consider the uniqueness of the upper JRS-Hessenberg reduction.

### 3.4.1 The uniqueness of the upper JRS-Hessenberg reduction

Let \(M\) be a JRS-symmetric matrix of order \(4n\) and let \(H = WMW^T\) be a orthogonally JRS-symmetric reduction of \(M\) to upper JRS-Hessenberg form. When reducing \(M\) to upper JRS-Hessenberg form \(H\) by a unitary similarity, we must introduce \(4(2n - 1)(n - 1)\) zeros but only \((n - 1)(n - 2)/2\) free zeros into \(M\). Notice that an orthogonally JRS-symmetric matrix has \(n(n - 1)/2\) degrees of freedom. Since we must use \((n - 1)(n - 2)/2\) of the degrees of freedom to introduce zeros in \(M\), we have \(n - 1\) degrees of freedom left over in \(W\), just enough to specify the first column of \(W\).

**Theorem 3.5 (Implicit Q Theorem for JRS-Hessenberg Form).** Suppose that \(M\) is a \(4n\times4n\) JRS-symmetric matrix, and \(U := [u_1, \ldots, u_{4n}]\) and \(V := [v_1, \ldots, v_{4n}]\) are orthogonally JRS-symmetric matrices such that \(U^T MU = H\) and \(V^T MV = \tilde{H}\) are upper JRS-Hessenberg forms defined by (3.3). Let \(r\) denote the smallest positive integer for which \(H_0(r, r - 1) = 0\), with the convention that \(r = n\) if \(H\) is unreduced. If \([u_1, u_{n+1}, u_{2n+1}, u_{3n+1}] = [v_1, v_{n+1}, v_{2n+1}, v_{3n+1}]\), then \([u_s, u_{n+s}, u_{2n+s}, u_{3n+s}] = \pm[v_s, v_{n+s}, v_{2n+s}, v_{3n+s}]\) for \(s = 2 : r\). Moreover, if \(r < n\), then \(H_0(r + 1, r) = 0\).

**Proof.** Define \(W = V^T U\) and two kinds of partitioning

\[
W := [w_1 \cdots w_{4n}] := \begin{bmatrix}
W_0 & W_2 & W_1 & W_3 \\
-W_2 & W_0 & W_3 & -W_1 \\
-W_1 & -W_3 & W_0 & W_2 \\
-W_3 & W_1 & -W_2 & W_0
\end{bmatrix}.
\]

Then \(W\) is orthogonally JRS-symplectic and

\[
[w_1, w_{n+1}, w_{2n+1}, w_{3n+1}] = [e_1, e_{n+1}, e_{2n+1}, e_{3n+1}].
\]

Denote that \(H := [h_1, \ldots, h_{4n}]\). The equation \(\tilde{H}W = WH\) implies that

\[
\tilde{H}[w_s, w_{n+s}, w_{2n+s}, w_{3n+s}] = W[h_s, h_{n+s}, h_{2n+s}, h_{3n+s}], s = 2, \cdots, n.
\]
So that
\[
[w_s, w_{n+s}, w_{2n+s}, w_{3n+s}] H_0(s, s - 1) = \hat{H}[w_{s-1}, w_{n+s-1}, w_{2n+s-1}, w_{3n+s-1}]
\]
\[- [W_{s,1}, W_{s,2}, W_{s,3}, W_{s,4}] \begin{bmatrix}
H_0(1 : s-1, s-1) & H_0(1 : s-1, s) & H_0(1 : s-1, 1) & H_0(1 : s-1, 0)
\- H_0(1 : s-1, s-1) & H_0(1 : s-1, s) & H_0(1 : s-1, 1) & H_0(1 : s-1, 0)
\- H_0(1 : s-1, s-1) & H_0(1 : s-1, s) & H_0(1 : s-1, 1) & H_0(1 : s-1, 0)
\- H_0(1 : s-1, s-1) & H_0(1 : s-1, s) & H_0(1 : s-1, 1) & H_0(1 : s-1, 0)
\end{bmatrix}
\]
where each \(W_{s,t} := W(:, (t-1)n + 1 : (t-1)n + s - 1)\), \(t = 1, \ldots, 4\). Since \(\hat{H}\) is upper JRS-Hessenberg matrix,
\[
\hat{H}[w_{s-1}, w_{n+s-1}, w_{2n+s-1}, w_{3n+s-1}] := \begin{bmatrix}
\hat{W}_0(:, s-1) & \hat{W}_2(:, s-1) & \hat{W}_4(:, s-1) & \hat{W}_6(:, s-1)
\- \hat{W}_2(:, s-1) & \hat{W}_0(:, s-1) & \hat{W}_2(:, s-1) & \hat{W}_4(:, s-1)
\- \hat{W}_4(:, s-1) & \hat{W}_2(:, s-1) & \hat{W}_0(:, s-1) & \hat{W}_2(:, s-1)
\- \hat{W}_6(:, s-1) & \hat{W}_4(:, s-1) & \hat{W}_2(:, s-1) & \hat{W}_0(:, s-1)
\end{bmatrix}
\]
is JRS-symmetric, where \(\hat{W}_0(:, s-1)\) has its last \(n - s\) entries being zeros and the \(s\)-th entry nonzero, \(\hat{W}_1(:, s-1)\) and \(\hat{W}_3(:, s-1)\) have their last \(n - s + 1\) entries being zeros. By introduction on \(n\), we can see that \(W_0(:, 1 : s)\) is upper triangular with nonzero entries on its diagonal, \(W_1(:, 1 : s)\), \(W_2(:, 1 : s)\) and \(W_3(:, 1 : s)\) are strictly upper triangular. Thus for \(2 \leq s \leq r\),
\[
[w_s, w_{n+s}, w_{2n+s}, w_{3n+s}] = \pm[e_s, e_{n+s}, e_{2n+s}, e_{3n+s}].
\]
Since \(U = VW\), we obtain
\[
[u_s, u_{n+s}, u_{2n+s}, u_{3n+s}] = \pm[v_s, v_{n+s}, v_{2n+s}, v_{3n+s}], \ s = 2, \ldots, r.
\]
Multiplying equation (3.2) by \(w_r^T\) from the left side, there is \(H_0(r, r - 1) = w_r^T \hat{H} w_{r-1}\), and then
\[
|H_0(r, r - 1)| = |u_r^T \hat{H} V V^T u_{r-1}| = |u_r^T M u_{r-1}| = |v_r^T M v_{r-1}| = |\hat{H}_0(r, r - 1)|.
\]
If \(r < n\), the structures of \(W\) and \(H\) implies
\[
\hat{H}_0(r, r - 1) = e_r^T \hat{H} e_r = \pm e_r^T M D e_r = \pm e_r^T W D e_r = W(r + 1, :) D(:, r)
\]
\[
= \begin{bmatrix}
W_0(r+1,:) & W_2(r+1,:) & W_4(r+1:)
\end{bmatrix}
\begin{bmatrix}
H_0(:, r)
\- H_2(:, r)
\- H_4(:, r)
\end{bmatrix} = 0.
\]
\]

An important result following the implicit Q theorem is that if both \(U^T MU = H\) and \(V^T MV = \hat{H}\) are unreduced upper JRS-Hessenberg matrices and \([u_1, u_{n+1}, u_{2n+1}, u_{3n+1}] = [v_1, v_{n+1}, v_{2n+1}, v_{3n+1}]\), then \(H\) and \(\hat{H}\) are “essentially equal” in the sense that \(\hat{H} = S^{-1} HS\) with \(S = \text{diag}(\pm 1, \ldots, \pm 1)\).

3.4.2 The double-implicit-shift strategy

We now return to our preliminary algorithm and modify it to avoid the expensive computation of \(H^2 - 2Re(\kappa)H + |\kappa|^2 I\). Let \(\kappa\) be a complex Francis shift of \(H\). If we compute the Q-factor \(\hat{W}\) of the matrix \(H^2 - 2Re(\kappa)H + |\kappa|^2 I\) then \(\hat{H} = \hat{W}^T H \hat{W}\) is the result of applying two steps of the QR algorithm with shifts \(\kappa\) and \(\tau\). The work of simultaneously determining \(\hat{W}\) and \(\hat{H}\) can be resolved into five steps:

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1. Compute the $1$, $n+1$, $2n+1$ and $3n+1$ columns of $C = H^2 - 2Re(\kappa)H + |\kappa|^2 I \in \mathbb{R}^{4n \times 4n}$, and save them into $F \in \mathbb{R}^{4n \times 4n}$.

2. Determine a Householder transformation $W_F \in \mathbb{R}^{4n \times 4n}$ such that
\[
W_F^T F = \sigma [e_1, e_{n+1}, e_{2n+1}, e_{3n+1}],
\]
where each $e_s$ denotes the $s$-th column of the identity matrix and $\sigma \in \mathbb{R}$ is nonnegative.

3. Set $H_F = W_F^T H W_F$.

4. Use Householder transformations to reduce $H_F$ to upper JRS-Hessenberg form $\hat{H}$. Call the accumulated transformations $\hat{W}$.

5. Set $\hat{W} = W_F \hat{W}$.

The key computations are the computation of the $1$, $n+1$, $2n+1$ and $3n+1$ columns of $C$ and the reduction of $H_F$ to upper JRS-Hessenberg form. Because $H$ is upper JRS-Hessenberg one can effect the first calculation in $O(1)$ operations and the second in $O(n^2)$ operations. We now turn to the details. For simplicity, if there is no confusion then a JRS-symmetric matrix is represented by its first block row, such as
\[
H := [H_0, H_2, H_1, H_3].
\]

**Remark 3.1.** A JRS-symmetric matrix is uniquely determined by its four submatrices on the first row block, and the converse is also true. The structure-preserving transformation on a JRS-symmetric matrix is equivalent to corresponding transformations on four submatrices on the first row block.

**Getting started.** Define $C = H^2 - 2Re(\kappa)H + |\kappa|^2 I := [C_0, C_2, C_1, C_3]$. The computation of the first column of $C_s (s = 0, 1, 2, 3)$ requires that we first compute the scalars $2Re(\kappa)$ and $|\kappa|^2$. To do this we need to compute $\kappa$ firstly. Define a submatrix of $H$ according to $m = n - 1$ as
\[
H_{mn} = \begin{bmatrix}
H_0(m : n, m : n) & H_2(m : n, m : n) & H_1(m : n, m : n) & H_3(m : n, m : n) \\
-H_2(m : n, m : n) & H_0(m : n, m : n) & -H_3(m : n, m : n) & H_1(m : n, m : n) \\
-H_1(m : n, m : n) & -H_3(m : n, m : n) & H_0(m : n, m : n) & -H_2(m : n, m : n) \\
-H_3(m : n, m : n) & H_1(m : n, m : n) & -H_2(m : n, m : n) & H_0(m : n, m : n)
\end{bmatrix},
\]
where each $H_s(m : n, m : n)$ denotes the submatrix on $m$ and $n$ rows and columns of $H_s$. Compute the smallest magnitude eigenvalues of $H_{mn}$, and choose it as the shift $\kappa$.

Define $H^2 := [H_0, H_2, H_1, H_3]$. Because $H$ is upper JRS-Hessenberg, only the first three
components of the first column of $\tilde{H}_s$ are nonzero, $s = 0, \ldots, 3$. They are calculated by

$$[	ilde{H}_0(1 : 3, 1), \tilde{H}_2(1 : 3, 1), \tilde{H}_1(1 : 3, 1), \tilde{H}_3(1 : 3, 1)] =$$

\[
\begin{bmatrix}
    h_{11}^{(0)} & h_{11}^{(2)} & h_{11}^{(1)} & h_{11}^{(3)} \\
    h_{12}^{(0)} & h_{12}^{(2)} & h_{12}^{(1)} & h_{12}^{(3)} \\
    h_{21}^{(0)} & h_{21}^{(2)} & h_{21}^{(1)} & h_{21}^{(3)} \\
    h_{32}^{(0)} & h_{32}^{(2)} & h_{32}^{(1)} & h_{32}^{(3)}
\end{bmatrix}
\begin{bmatrix}
    \tilde{h}_{11}^{(0)} & \tilde{h}_{11}^{(2)} & \tilde{h}_{11}^{(1)} & \tilde{h}_{11}^{(3)} \\
    \tilde{h}_{12}^{(0)} & \tilde{h}_{12}^{(2)} & \tilde{h}_{12}^{(1)} & \tilde{h}_{12}^{(3)} \\
    \tilde{h}_{21}^{(0)} & \tilde{h}_{21}^{(2)} & \tilde{h}_{21}^{(1)} & \tilde{h}_{21}^{(3)} \\
    \tilde{h}_{32}^{(0)} & \tilde{h}_{32}^{(2)} & \tilde{h}_{32}^{(1)} & \tilde{h}_{32}^{(3)}
\end{bmatrix}.
\]

Then the first column of $C_s$ is

$$c_s = C_s(:, 1) = \begin{bmatrix} \tilde{H}_s(1 : 3, 1) - 2\text{Re}(\kappa)H_s(1 : 3, 1) + |\kappa|^2I(1 : 3, sn + 1) \\ 0 \\ \vdots \\ 0 \end{bmatrix}, s = 0, \ldots, 3.$$

(3.11)

Now we apply the substitution of $t$ for $2\text{Re}(\kappa)$ and $d$ for $|\kappa|^2$ to make sure that our algorithm works even if the Francis double shifts are real. Specifically, suppose that the matrix $H_{mn}$ has two smallest magnitude eigenvalues $\lambda$ and $\mu$. Then

$$C = (H - \lambda I)(H - \mu I) = H^2 - (\lambda + \mu)H + \lambda \mu I = H^2 - tH + dI.$$

Then we collect the first columns of $C_0, \ldots, C_3$ in

$$F := [c_0, c_2, c_1, c_3] = \begin{bmatrix} f_0 & f_2 & f_1 & f_3 \\ 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

with

$$f_s = \tilde{H}_s(1 : 3, 1) - tH_s(1 : 3, 1) + dI(1 : 3, sn + 1) \in \mathbb{R}^3, s = 0, \ldots, 3.$$

Observe that the Household transformation $W_F$ such that $W_F^T F := \sigma[c_1, 0, 0, 0]$ can be determined in $O(1)$ flops.

**Reduction back to JRS-Hessenberg form.** Since a similarity transformation with $W_F$ only changes the first, second and third rows and columns of $H_s$, so that $H_F = W_F^T H W_F$ has the form

$$H_F = \begin{bmatrix}
    H_0^F & H_2^F & H_1^F & H_3^F \\
    -H_2^F & H_0^F & H_2^F & -H_3^F \\
    -H_1^F & -H_2^F & H_1^F & H_3^F \\
    -H_3^F & H_1^F & -H_2^F & H_0^F
\end{bmatrix}$$

(3.13)
where
\[
H_0^F = \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & x & x \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix},
\quad H_{1,2,3}^F = \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & x \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
\]

This matrix can be restored to upper JRS-Hessenberg form by the orthogonally JRS-symplectic transformations. The calculation proceeds are as follows:

\[
[H_0^F, H_2^F, H_1^F, H_3^F] \xrightarrow{\mathbf{W}_1} \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\xrightarrow{\mathbf{W}_2} \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\xrightarrow{\mathbf{W}_3} \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

\[
\xrightarrow{\mathbf{W}_4} \begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]
3.4.3 Computing the real JRS-Schur form

The standard way to solve the dense nonsymmetric eigenproblem is firstly reducing a matrix to the upper Hessenberg form, and producing the real Schur form by iteration with the Francis QR step. In this subsection we indicate how to reduce a real JRS-Hessenberg matrix $H$ to a real JRS-Schur form $T$. Now we prove that the upper JRS-Hessenberg structure is preserved through the shift QR iteration.

**Theorem 3.6.** Suppose $H \in \mathbb{R}^{4n \times 4n}$ is unreduced upper JRS-Hessenberg, and $\kappa \in \mathbb{C}$ does not represent an eigenvalue of $H$. If $WR = C := H^2 - 2\text{Re}(\kappa)H + |\kappa|^2I$ is a JRS-QR decomposition, then $\hat{H} = W^THW$ is also upper JRS-Hessenberg.

*Proof.* Since $\kappa$ is not an eigenvalue of $H$, $C$ is nonsingular, and so is $R$. The orthogonally JRS-symplectic matrix $W = CR^{-1}$, and $W^T = W^{-1} = RC^{-1}$. Since $CH = HC$, $W^THW = RC^{-1}HCR^{-1} = RHR^{-1}$. Note that $R$ and $R^{-1}$ are JRS-triangular. As the product of two JRS-triangular matrices with a JRS-Hessenberg matrix, $\hat{H}$ is upper JRS-Hessenberg. \qed

The implicit determination of $\hat{H}$ from $H$ outlined above bases on the Francis QR step, first described by Francis (1961) and then included in the books [10, 28].

### 3.4.3 Computing the real JRS-Schur form

The standard way to solve the dense nonsymmetric eigenproblem is firstly reducing a matrix to the upper Hessenberg form, and producing the real Schur form by iteration with the Francis QR step. In this subsection we indicate how to reduce a real JRS-Hessenberg matrix $H \in \mathbb{R}^{4n \times 4n}$ to a real JRS-Schur form $T = W^THW$ with the orthogonal JRS-symplectic matrix $W$.

Denote that $H := [H_0, H_2, H_1, H_3]$, $W := [W_0, W_2, W_1, W_3]$ and $T := [T_0, T_2, T_1, T_3]$.

- Firstly, find the largest nonnegative integer $q$ and the smallest nonnegative integer $p$ such that

  $H_0 = \begin{bmatrix}
  H_{11} & H_{12} & H_{13} \\
  0 & H_{22} & H_{23} \\
  0 & 0 & H_{33}
  \end{bmatrix}
  \begin{bmatrix}
p \\
n - p - q \\
q
  \end{bmatrix}$

  where $H_{33}$ is upper quasi-triangular and $H_{22}$ is unreduced.

- Secondly, if $q < n$, perform a Francis JRS-QR step on the unreduced upper JRS-Hessenberg matrix $H_{22}$:

  $H_{22} = \hat{W}^TH_{22}\hat{W}$.

Let $\epsilon$ denote the machine precision. The calculated real JRS-Schur form $\hat{T}$ has the structure defined by (3.8) and is orthogonally similar to a JRS-symmetric matrix near to $H$, i.e.,

$W^T(H + E)W = \hat{T},$

where $W$ is orthogonally JRS-symplectic, $E$ is JRS-symmetric with small $\|E\|_2 \approx \epsilon\|H\|_2$. The calculated $\hat{W}$ is almost orthogonally JRS-symplectic in the sense that $\hat{W}^T\hat{W} - I = F$ is JRS-symplectic and $\|F\|_2 \approx \epsilon$. 

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Recall the observation in Theorem 2.2 that the structure-preserving decompositions of $JRS$-symmetric matrices can lead to the corresponding decompositions of quaternion matrices. For instance, the upper $JRS$-Hessenberg form $H$ defined by (3.3) is a real counterpart of quaternion matrix $H_0 + H_1i + H_2j + H_3k$, which is a quaternion Hessenberg matrix with real subdiagonal elements; and the orthogonally $JRS$-symplectic matrix $W$ defined by (3.1) is a real counterpart of a unitary quaternion matrix $W_0 + W_1i + W_2j + W_3k$. The QR, block-diagonal Schur and Hessenberg decompositions of quaternion matrices can be easily elicited from those of $JRS$-matrices based on Theorem 2.2. One of the most important improvements here is that the subdiagonal (or diagonal) entries of Hessenberg and block-diagonal Schur forms (or $R$-factor) are real numbers, which will greatly enhance the algorithms based on quaternion matrix decompositions.

4 A new implicit double shift quaternion QR algorithm

In this section, we present a new fast quaternion QR algorithm with applying the real structure-preserving methods.

A strategy to solve the eigenproblem of a general quaternion matrix $Q \in \mathbb{H}^{n \times n}$ can be described in two steps:

1) Calculate the real $JRS$-Schur form (3.8) of the real counterpart $\Upsilon_Q \in \mathbb{R}^{4n \times 4n}$ of $Q$, and then lead to the quasi upper-triangular Schur matrix

$$T = T_0 + T_1i + T_2j + T_3k \in \mathbb{H}^{n \times n},$$

where $T_0 \in \mathbb{R}^{n \times n}$ is a real Schur form, $T_1, T_2$ and $T_3 \in \mathbb{R}^{n \times n}$ are upper triangular.

2) Solve the eigenproblem of $T$ and backstep for eigen-information of $Q$ under similarity transformations.

We will concentrate into the first step to develop a new version of the practical quaternion QR algorithm in [1]. Without causing any confusion, we use the same notation $[Q_0, Q_2, Q_1, Q_3]$ to represent the quaternion matrix $Q = Q_0 + Q_1i + Q_2j + Q_3k$, $Q_0, \ldots, Q_3 \in \mathbb{R}^{n \times n}$, and its real counterpart $\Upsilon_Q \in \mathbb{R}^{4n \times 4n}$. See Remark 3.1 for the explanation.

4.1 Basic quaternion operations

At first we introduce several unitary quaternion transformations, including four improved Householder-based transformations and one generalized quaternion Givens transformation.

4.1.1 Improved Householder-based transformations

Four Householder-based transformations proposed in [1, 24, 15, 21] are recalled with slight improvement.

Given two different quaternion vectors $x = [x_1, \ldots, x_n]^T$, $y = [y_1, \ldots, y_n]^T \in \mathbb{H}^n$ with $\|x\| = \|y\|$ and $y^*x \in \mathbb{R}$, there exists a quaternion Householder matrix defined by $H = I - 2uu^*$,
where \( u = \frac{y-x}{\|y-x\|} \), such that \( H y = x \); see \cite{1} and \cite{21} Theorem 3.1 and Theorem 3.2. Applying real structure-preserving methods, we can execute four kinds of improved Householder-based transformations: for any real vector \( v \in \mathbb{R}^n \) with \( \|v\| = 1 \),

- when \( x = \alpha v \) with \( \alpha \in \mathbb{H} \) and \( |\alpha| = \|y\| \), \( H_1 := I - 2uu^* \), where \( u = \frac{y-x}{\|y-x\|} \), (proposed in \cite{1})
- when \( x = \|y\|v \), \( H_2 := \frac{1}{\xi}(I - uu^*) \), where \( u = \frac{y - \xi x}{\sqrt{\|y\|(\|y\| + \|y^T v\|)}} \), \( \xi = \begin{cases} 1, & |y^T v| = 0, \\ -\frac{T}{|y^T v|}, & \text{otherwise}, \end{cases} \)
  (proposed in \cite{15})
- when \( x = \|y\|v \), \( H_3 := (I - 2uu^T)G \), where \( u = \frac{G(y-x)}{\|G(y-x)\|} \), \( G = \text{diag}(g_1, g_2, \ldots, g_n) \),
  \( g_\ell = \begin{cases} \frac{z_\ell}{|z_\ell|}, & z_\ell \neq 0, \\ 1, & \text{otherwise}, \end{cases} \)
  (proposed in \cite{21})
- and when \( x = \|y\|v \), \( H_4 := G H_1 \), where \( G = \text{diag}(g_1, g_2, \ldots, g_n) \),
  \( g_\ell = \begin{cases} \frac{z_\ell}{|z_\ell|}, & z_\ell \neq 0, \\ 1, & \text{otherwise} \end{cases} \)
  with \( z = H_1 y \).

**Remark 4.1.** If \( v \) is one column of the identity matrix, then \( H_2 = H_4 = g H_1 \), where \( g \) is a unit quaternion scalar which rotates the nonzero element of \( H_1 y \) into a positive number.

**Remark 4.2.** As pointed by Li et al. \cite{21}, \( H_1, \ldots, H_4 \) are unitary quaternion matrices and only \( H_1 \) is Hermitian and reflective.

**Remark 4.3.** Applying the realization of the quaternion operations in Section 2.1, we can execute the quaternion Householder-based transformations in real arithmetic. The necessary real flops and assignment numbers are listed in Table 1.

### 4.1.2 Generalized quaternion Givens transformations

Janovská and Opfer extended the Givens transformation to quaternion valued matrices in \cite{17}. Recall \cite{17} Theorem 3.4 that for given nonzero vector \( x = [x_1, x_2]^T \in \mathbb{H}^2 \), define

\[
G_1 = \begin{bmatrix} \bar{\sigma} & s \\ -\bar{c} & c \end{bmatrix}, \quad \text{with} \quad s = -\sigma \frac{x_2}{\|x\|}, \quad c = \sigma \frac{x_1}{\|x\|}, \quad |\sigma| = 1,
\]

where \( \sigma \) is arbitrary in case \( x_1, x_2 \) are linearly dependent over \( \mathbb{R} \) or otherwise \( \sigma = \frac{\alpha x_1 + \beta x_2}{\|\alpha x_1 + \beta x_2\|} \in \mathbb{H} \) with nonzero vector \( [\alpha, \beta]^T \in \mathbb{R}^2 \), then \( G_1 \) is a unitary matrix and \( G_1^* x = \sigma [\|x\|, 0]^T \). Their extension is based on the traditional form of Givens matrix. We will define a new quaternion Givens transformation in a different view from \cite{17} \cite{15}.
Table 1: Computation amounts and assignment numbers for $H_\ell$ and $H_\ell x$.

| Methods | Generate matrix $H_\ell$ assignment | Transformation $H_\ell x$ assignment | real flops | real flops |
|---------|----------------------------------|----------------------------------|------------|------------|
| $H_1$  | 8  | 8\(n + 19\) | 2  | 80\(n - 4\) |
| $H_2$  | 10 | 8\(n + 30\) | 4  | 80\(n + 24\) |
| $H_3$  | \(n + 1\) | 13\(n + 2\) | 2\(n + 2\) | 32\(n\) |
| $H_4$  | 10 | 8\(n + 30\) | 4  | 80\(n + 24\) |

**Theorem 4.1.** Let $x = [x_1 \ x_2]^T \in \mathbb{H}^2$ be given with $x_2 \neq 0$. Then there exists a generalized Givens matrix $G_2 = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$ such that $G_2^* x = [\|x\|_2 \ 0]^T$. A choice of $G_2$ is

\[
g_{11} = \frac{x_1}{\|x\|_2}, \quad g_{21} = \frac{x_2}{\|x\|_2};
\]

if $|x_1| \leq |x_2|$, $g_{12} = |g_{21}|$, $g_{22} = -|g_{21}|g_{22}^*$; \hspace{1cm} (4.1)

if $|x_1| > |x_2|$, $g_{22} = |g_{11}|$, $g_{12} = -|g_{11}|g_{12}^*$.

**Proof.** Because $G_2$ is required to be unitary, we can define

\[
g_{11} = \frac{x_1}{\|x\|_2}, \quad g_{21} = \frac{x_2}{\|x\|_2},
\]

and $g_{12}, g_{22}$ should satisfy

\[
g_{11}^* g_{12} + g_{21}^* g_{22} = 0, \quad g_{12}^* g_{12} + g_{22}^* g_{22} = 1. \hspace{1cm} (4.2)
\]

In order to ensure stability, the selection problem of $g_{12}, g_{22}$ will be discussed in the following two cases.

(1) $|x_1| \leq |x_2|$ if and only if $|g_{11}| \leq |g_{21}|$. From (4.2), we get

\[
g_{22} = -g_{21}^* g_{12}, \quad 1 = |g_{12}|^2 + |g_{21}|^2 |g_{22}^* g_{11}|^2.
\]

Then we can choose

\[
g_{12} = \frac{1}{\sqrt{1 + |g_{21} g_{11}|^2}} = \frac{1}{\sqrt{1 + |g_{21}|^2 |g_{11}|^2}} = \frac{|g_{21}|}{\sqrt{|g_{21}|^2 + |g_{11}|^2}} = |g_{21}|,
\]

and then

\[
g_{22} = -|g_{21}| g_{21}^* g_{11}.
\]

(2) $|x_1| > |x_2|$ if and only if $|g_{11}| > |g_{21}|$. From (4.2), we get

\[
g_{12} = -g_{11}^* g_{21} g_{22}, \quad 1 = g_{12}^* g_{12} + g_{22}^* g_{22} = |g_{22}|^2 |g_{11}^*|^2 |g_{21}|^2 + |g_{22}|^2.
\]
Table 2: Computation amounts and assignment numbers for quaternion Givens Transformations.

| Methods                        | Generate $G$ assignment | Givens Transformation $G^*x$ assignment | real flops | real flops |
|--------------------------------|-------------------------|-----------------------------------------|------------|------------|
| Fast Quaternion Givens $G_1$   | 15                      | 2                                       | 120        | 120        |
| Generalized Quaternion Givens $G_2$ | 9                      | 2                                       | 69         | 120        |

Therefore we can choose

$$g_{22} = \frac{1}{\sqrt{1 + |g_{11}^{-1}|^2|g_{21}|^2}} = \frac{|g_{11}|}{\sqrt{|g_{11}|^2 + |g_{21}|^2}} = |g_{11}|,$$

and then

$$g_{12} = -|g_{11}|g_{11}^{-1}g_{21}^*.$$

Obviously, $G_2$ with such structure is unitary. Finally,

$$G_2^*x = \sqrt{||x||_2},0)^T.$$

**Remark 4.4.** The quaternion Givens matrix $G_2$ is the generalization of real Givens matrix, and $|g_{11}| = |g_{22}|, |g_{21}| = |g_{12}|$.

**Remark 4.5.** According to the absolute value of $x_1, x_2$, we take the different $g_{12}, g_{22}$. When $|x_1| \leq |x_2|$, then $|g_{12}| = |g_{21}| \geq \sqrt{2}$. It can ensure stability in the process of computing $g_{22}$. When $|x_1| > |x_2|$, then $|g_{22}| = |g_{11}| > \sqrt{2}$. It can ensure stability in the process of computing $g_{21}$.

**Remark 4.6.** In Table 2, we present the comparison on the computation amounts and assignment numbers between the generalized quaternion Givens transformations and the fast quaternion Givens transformations.

4.2 The quaternion Hessenberg reduction

The Hessenberg reduction of quaternion matrices based on quaternion Householder-based transformations were firstly proposed in [1] in the range of our knowledge.

Reducing a quaternion matrix $Q \in \mathbb{H}^{n \times n}$ to the Hessenberg form means to find a unitary quaternion matrix $W = W_0 + W_1i + W_2j + W_3k$ such that

$$W^*QW = H,$$

where $H = H_0 + H_1i + H_2j + H_3k, H_0, \ldots, H_3 \in \mathbb{R}^{n \times n}$ are upper Hessenberg matrices. Since the real counterpart of $Q$ is JRS-symmetric, we can firstly calculate the JRS-Hessenberg form

$$W^*W = H,$$

and then

$$W^*QW = H.$$
$H$ of $\mathcal{H}$ as shown in the proof of Theorem \ref{thm:main} and then backstep for the Hessenberg form of the quaternion matrix by Theorem \ref{thm:backstep}.

Now we present three real structure-preserving algorithms. For simplicity, we need to define two auxiliary functions:

$$\text{id}(p) = [p, n+p, 2n+p, 3n+p] , \text{ in}(p, q) = [p : q, n+p : n+q, 2n+p : 2n+q, 3n+p : 3n+q]$$ \hspace{1cm} (4.4)

for any positive integers $p$ and $q$.

**Algorithm 4.1 (Quaternion Hessenberg Reduction Based on $\mathcal{H}_1$).** Given a quaternion matrix $Q = Q_0 + Q_1i + Q_2j + Q_3k \in \mathbb{H}^{n \times n}$, this algorithm overwrites $Q$ with an upper Hessenberg quaternion matrix $H = H_0 + H_1i + H_2j + H_3k$ satisfying $H = W^*QW$, where $W$ is a unitary quaternion matrix.

1. Form $H = [Q_0; Q_1; Q_2; Q_3]$;
2. for $s=2:n-1$
   3. $[u, \beta] = \mathcal{H}_1(H(\text{in}(s,n), s-1))$;
   4. $Y = H(\text{in}(s,n), s-1 : n)$;
   5. $H(\text{in}(s,n), s-1 : n) = Y - (\beta * u) * (u' * Y)$;
   6. $Y = [H(1 : n, s : n), -H(n+1 : 2n, s : n), -H(2n+1 : 3n, s : n),... -H(3n+1 : 4n, s : n)]$;
   7. $Y = Y - (Y * u) * (\beta * u')$;
   8. $H(:, s : n) = [Y(1 : n, 1 : n+1-s); Y(1 : n, nn+1 : 2(n+1-s));... -Y(1 : n, 2(n+1-s) + 1 : 3(n+1-s)); -Y(1 : n, 3(n+1-s) + 1 : 4(n+1-s))]$;
9. end

**Algorithm 4.2 (Quaternion Hessenberg Reduction Based on $\mathcal{H}_2$ or $\mathcal{H}_3$).** Given a quaternion matrix $Q = Q_0 + Q_1i + Q_2j + Q_3k \in \mathbb{H}^{n \times n}$, this algorithm overwrites $Q$ with an upper Hessenberg quaternion matrix $H = H_0 + H_1i + H_2j + H_3k$ satisfying $H = W^*QW$, where $W$ is a unitary quaternion matrix.

1. Run Algorithm 4.1 and store the computed upper Hessenberg matrix as $H := [H_0, H_2, H_1, H_3]$;
2. for $s=2:n$
  3. $G = JRSGivens(H(\text{id}(s+1), s));$ \hspace{1cm} (see \cite[Algorithm 3.3]{algorithm})
  4. $[H_0(t, s : n), H_2(t, s : n), H_1(t, s : n), H_3(t, s : n)]$
     \hspace{1cm} $= G^T[H_0(t, s : n); -H_2(t, s : n); -H_1(t, s : n); -H_3(t, s : n)];$
  5. $[H_0(:, t), H_2(:, t), H_1(:, t), H_3(:, t)] = [H_0(:, t), H_2(:, t), H_1(:, t), H_3(:, t)]G;
ALGORITHM 4.3 (Quaternion Hessenberg Reduction Based on $\mathcal{K}_3$). Given a quaternion matrix $Q := [Q_0, Q_2, Q_1, Q_3]$, where $Q_{0,2,3} \in \mathbb{R}^{n \times n}$, this algorithm overwrites $Q$ with an upper Hessenberg quaternion matrix $H := [H_0, H_2, H_1, H_3]$ satisfying $\Upsilon_H = \Upsilon_{W}^T \Upsilon_{Q} \Upsilon_{W}$, where $W := [W_0, W_2, W_1, W_3]$ is a unitary quaternion matrix.

1. for $s = 1 : n - 1$
2. for $t = s + 1 : n$
3. \[
G = \text{JRSGivens}(Q_0(t, s), Q_1(t, s), Q_2(t, s), Q_3(t, s)); \quad \text{(see } \textbf{Algorithm 3.3} \text{)}
\]
4. \[
[Q_0(t, s : n), Q_2(t, s : n), Q_1(t, s : n), Q_3(t, s : n)]
= G^T[Q_0(t, s : n); -Q_2(t, s : n); -Q_1(t, s : n); -Q_3(t, s : n)];
\]
5. \[
[Q_0(:, t), Q_2(:, t), Q_1(:, t), Q_3(:, t)] = [Q_0(:, t), Q_2(:, t), Q_1(:, t), Q_3(:, t)]G;
\]
6. end
7. if $s < n - 1$
8. \[
[u, \beta] = \text{house}(Q_0(s + 1 : n, s));
\]
9. \[
Q_{0,1,2,3}(s + 1 : n, s : n) = (I - \beta uu^T)Q_{0,1,2,3}(s + 1 : n, s : n);
\]
10. \[
Q_{0,1,2,3}(:, s + 1 : n) = Q_{0,1,2,3}(:, s + 1 : n)(I - \beta uu^T);
\]
11. end
12. end

In line 3 of Algorithm 4.2 and Algorithm 4.3 running the function JRSGivens costs 11 flops including in 1 square root operation. The transformation $G$ acts as a four-dimensional Givens rotation [7]. We refer to [22, 30] for a backward stable implementation of the generalized symplectic Givens rotation (3.2) and more Givens-like actions.

REMARK 4.7. With the same aim of executing the quaternion Hessenberg reduction in real arithmetic, Algorithms 4.1 and 4.3 are respectively based on the Householder-based transformations $\mathcal{K}_1$ and $\mathcal{K}_3$. The marked difference between them is in the following two aspects.

- They utilize different real counterparts of quaternion matrices: the real counterpart used in Algorithm 4.3 is defined as in (2.1), while that in Algorithm 4.7 is defined as

\[
\tilde{\Upsilon}_Q = \begin{bmatrix}
Q_0 & -Q_1 & -Q_2 & -Q_3 \\
Q_1 & Q_0 & -Q_3 & 0 \\
Q_2 & Q_3 & Q_0 & -Q_1 \\
Q_3 & -Q_2 & Q_1 & Q_0
\end{bmatrix}.
\] (4.5)

These two real counterparts are similar to each other and have the same functionality.

- They adopt different styles of data motion: the loads and stores of data are transported by four $n$-by-$n$ matrices in Algorithm 4.3, while in Algorithm 4.7 by one $4n$-by-$n$ matrices.
Table 3: Computation amounts and assignment numbers for Hessenberg reduction

| Householder | Dense Matrix $Q$ assignment | Dense Matrix $Q$ real flops | Broken Hessenberg matrix $H_F$ assignment | Broken Hessenberg matrix $H_F$ real flops |
|-------------|-----------------------------|----------------------------|------------------------------------------|------------------------------------------|
| $H_1$       | $9n - 12$                   | $128n^3/3$                 | $8n - 9$                                 | $188n^2$                                 |
| $H_2$ or $H_4$ | $14n - 17$                 | $184n^3/3$                 | $13n - 14$                               | $272n^2$                                 |
| $H_3$       | $8n^2 + 5n - 26$           | $80n^3/3$                  | $64n - 121$                              | $128n^2$                                 |

**Remark 4.8.** Algorithms [4.1, 4.3] are real structure-preserving methods with calculating the quaternion Hessenberg matrix defined in [1]. The calculated quaternion Hessenberg matrix by Algorithm 4.1 as well as that in [1] has quaternion elements on the subdiagonal; meanwhile, the calculated quaternion Hessenberg matrices by Algorithms 4.2 and 4.3 have positive real numbers on the subdiagonals. Algorithm 4.2 is the same as Algorithm 4.1 but with an additional step of rotating the quaternion elements on the subdiagonal to positive real numbers. Computation amounts numbers for the Hessenberg reduction of dense quaternion matrices are listed in the first two columns of Table 3.

**Remark 4.9.** In Algorithm 4.1 (lines 4-7), we have improved the line 3 of Algorithm 4.5 in [21] for multiplication by Householder matrices by reducing data motion. Remind that data motion is an important factor when reasoning about performance.

### 4.3 Quaternion Hessenberg QR

According to the conventional QR iteration method, the practical QR algorithm of quaternion matrices can be presented as

**Algorithm 4.4** (Practical Quaternion QR Algorithm). *Input quaternion matrix $Q = Q_0 + Q_1i + Q_2j + Q_3k \in \mathbb{H}^{n \times n}$.*

1. Preliminarily reduce $Q$ to the Hessenberg form $H$ (e.g., by Algorithm 4.3).
2. Until convergence, run

   Factor $H = WR$;

   Set $H = RW$.

In general case, the subdiagonal entries of $H$ tends to zero when proceeding the iteration. The main work is the QR factorization of the upper Hessenberg matrix $H$.

Now we reduce a quaternion Hessenberg matrix into a triangular quaternion matrix by unitary transformations based on the generalized quaternion Givens matrices.

**Algorithm 4.5** (Quaternion Hessenberg QR). *Given an upper Hessenberg quaternion matrix $H := [H_0, H_2, H_1, H_3]$, where $H_{0,1,2,3} \in \mathbb{R}^{n \times n}$, the following algorithm overwrites $H$ with an upper triangular quaternion matrix $R := [R_0, R_2, R_1, R_3]$ which satisfies $Y_R = Y_W^T Y_H$, where $W := [W_0, W_2, W_1, W_3]$ is a unitary quaternion matrix.*
1. for s=1:n-1
2. \( x := H([s, s + 1], [s, 2*n + s, n + s, 3*n + s]); \)
3. calculate the generalized quaternion Givens matrix \( G_2 \) as in Theorem 4.1;
4. \( H([s, s + 1], [s, 2*n + s, n + s, 3*n + s]) = G_2^* H([s, s + 1], [s, 2*n + s, n + s, 3*n + s]); \)
5. end

In Algorithm 4.5, \( n - 1 \) generalized quaternion Givens matrices are calculated. It needs 69 real flops and 3 square root operations to generate each \( G_2 \) by equation (4.1) if \( x_1 \) and \( x_2 \) are quaternion numbers. Notice that if \( x_2 \) is real, at most 48 flops (at least 33 flops) can be saved. This means if the inputting quaternion Hessenberg matrix has real subdiagonal entries (i.e., \( H_0 \) is of upper Hessenberg form and \( H_{1,2,3} \) are upper triangular), then the amount of calculation can be saved. So the cost of Algorithm 4.5 is about \( 120n^2 \) for a quaternion Hessenberg matrix of order \( n \). If we use fast quaternion Givens transformations instead of the generalized quaternion Givens transformations in line 3 of Algorithm 4.5, the cost of per iteration will rise to about \( 148n^2 \) for a quaternion Hessenberg matrix of order \( n \).

4.4 The implicit double shift quaternion QR algorithm

To ensure rapid convergence of quaternion QR algorithm, we need to shift the eigenvalue. Bunse-Gerstner, Byers and Mehrmann [1] pointed that the single-shift technique cannot choose any nonreal quaternion as the shift because of noncommutativity of quaternions and directly proposed the implicitly double shift QR algorithm. They proposed the implicitly double shift QR algorithm directly.

**Algorithm 4.6 (Implicitly Double Shift Quaternion QR Algorithm [1]).** Given a quaternion matrix \( A \in \mathbb{H}^{n \times n} \), set \( A_0 := U_0^* A U_0 \) where \( U_0 \) is unitary chosen so that \( A_0 \) is Hessenberg. For \( s = 0, 1, 2, \ldots \)

1. Select an approximate eigenvalue \( \mu \in \mathbb{H} \).
2. Set \( A_{k+1} := Q_k^* A_k Q_k \) where \( Q_k \) is unitary chosen so that \( Q_k^* (A_k^2 - (\mu + \overline{\mu}) A_k + \mu \overline{\mu}) \) is triangular.

Generally, the \( A_k^2 - (\mu + \overline{\mu}) A_k + \mu \overline{\mu} \) can not be explained as \( (A_k - \mu I)(A_k - \overline{\mu} I) \) when the shift \( \mu \) is a nonreal quaternion number.

In this section, we firstly introduce the implicitly double shift JRS-QR algorithm for calculating real JRS-Schur forms of real counterparts of quaternion matrices, and then propose a new and fast implicit double shift quaternion QR algorithm. Based on the real structure-preserving methods, the double shift technique is applied to the real counterpart instead of quaternion matrix itself and the dimension is not expanded.

4.4.1 The implicitly double shift JRS-QR algorithm

Once the upper Hessenberg reduction is completed, the calculation of the real JRS-Schur form by the Francis QR step becomes the main step of solving the dense unsymmetric eigenproblem.

Firstly, we present the Francis JRS-QR step on the unreduced upper JRS-Hessenberg matrix \( H \).
Algorithm 4.7 (Francis JRS-QR step). Given the unreduced upper JRS-Hessenberg matrix $H \in \mathbb{R}^{4n \times 4n}$ and $s, t \in \mathbb{R}$, this algorithm overwrite $H$ with $W_F^T H W_F$, where $W_F$ is an orthogonal JRS-symplectic matrix.

1. $m=n-1$;
2. $F=H(:,1,3,:)*H(:,1,3)-s*H(:,1,3,:)+t*[1;0;0,0,0]$; (see definitions in [4.3])
3. for $k=1:n-2$
4. $W_F = \text{house}(F)$; (the function house is defined by (3.7))
5. $q=\max(1,k-1)$;
6. $H(:,1,k+2,:),\in(q,n))=W_F^T *H(:,1,k+2,:),\in(q,n))$;
7. $r=\min(k+3,n)$;
8. $H(:,1,r,:),\in(k,k+2))= H(:,1,r,:),\in(k,k+2)) *W_F$;
9. if $k < n-2$
10. $F=H(:,k+1,k+3,:),\id(k))$;
11. end
12. end
13. $W_F = \text{house}(H(:,n-1,n,:),\id(n-2))$;
14. $H(:,n-1,n,:),\in(n-2,n))=W_F^T *H(:,n-1,n,:),\in(n-2,n))$;
15. $H(:,n-2,n,:),\in(n-1,n))= H(:,n-2,n,:),\in(n-1,n)) *W_F$;
16. $W_F = \text{house}(H(:,n-1,n,:),\id(n-1))$;
17. $H(:,n-1,n,:),\id(n-1))=W_F^T *H(:,n-1,n,:),\id(n-1))$;
18. $H(:,n-2,n,:),\id(n))= H(:,n-2,n,:),\id(n)) *W_F$;

This algorithm requires $138n^2$ flops. If $W_F$ is accumulated into a given orthogonal matrix, additional $138n^2$ flops are necessary. Steps 16-18 are to delete the nonzero $(n, n-1)$-element of $H_1$, $H_2$ and $H_3$. Algorithm 4.7 can preserve the upper JRS-Hessenberg form defined by (3.1). Notice that if we use the MATLAB order hess on $M$, the resulted Hessenberg form is not JRS-symmetric.

Remark 4.10. In Algorithm 4.7, we are in essence processing the Hessenberg reduction of the broken quaternion Hessenberg matrix, of which the submatrix of first four rows and three columns no longer has upper Hessenberg form. Since only two elements are need to be cancelled, the Householder matrix is 3-by-3, and so the processing totally needs $O(n^2)$ flops. The computational counts are listed in the last two columns of Table 3.

During the iteration in Francis JRS-QR step, it is necessary to monitor the subdiagonal elements in $H_0$ in order to spot any possible decoupling. We illustrate how to do this in the following algorithm.
**Algorithm 4.8 (Real JRS-Schur form of a real upper JRS-Hessenberg matrix).**

Given a real upper JRS-Hessenberg matrix \( H \in \mathbb{R}^{n \times n} \) and a tolerance \( \text{tol} \) greater than the unit roundoff, this algorithm computes the real JRS-Schur canonical form \( W^T HW = T \), where \( W \) is orthogonally JRS-symplectic.

1. while \( q < n \)
   
   2. Set to zero all subdiagonal elements of \( H_0 = H(1:n, 1:n) \) that satisfy:
      
      \[ |H_0(i, i-1)| < \text{tol}(\|H(i, \text{id}(i-1))\|_2 + \|H(i-1, \text{id}(i))\|_2); \]

   3. Find the largest nonnegative integer \( q \) and the smallest non-negative integer \( p \) such that
      
      \[
      H_0 = \begin{bmatrix}
      H_{11} & H_{12} & H_{13} \\
      0 & H_{22} & H_{23} \\
      0 & 0 & H_{33}
      \end{bmatrix}
      \]

      where \( H_{33} \) is upper quasi-triangular and \( H_{22} \) is unreduced.

   4. If \( q < n \), perform a Francis JRS-QR step (Algorithm 4.7) on the unreduced upper JRS-Hessenberg matrix \( H((n)\text{in}(p+1,n-q), \text{in}(p+1,n-q))): \)
      
      \[
      \begin{align*}
      H(\text{in}(p+1,n-q), \text{in}(p+1,n-q)) & = W_F^T H(\text{in}(p+1,n-q), \text{in}(p+1,n-q))W_F, \\
      H(1:p, \text{in}(p+1:n-q)) & = H(1:p, \text{in}(p+1:n-q))W_F, \\
      H(p+1:n-q, \text{in}(n-q+1,n)) & = W_F^T H(p+1:n-q, \text{in}(n-q+1,n)).
      \end{align*}
      \]

5. end

Based on the empirical observation that average only two Francis iterations are required before the lower 1-by-1 or 2-by-2 decouples, this algorithm approximately requires \( 106\frac{2}{3}n^3 \) flops if only the eigenvalues are desired. If \( W \) and \( T \) are computed, then \( 325\frac{4}{7}n^3 \) flops are necessary.

**Remark 4.11.** If we use the traditional Francis QR step instead of the Francis JRS-QR step in line 4, then the flops count for computing \( T \) and \( W \) will rise to \( 1600n^3 \). It is worse that \( W \) and \( T \) will no longer be JRS-symmetric and the storage space will be multiplied four times.

### 4.4.2 Implicitly Double Shift Quaternion QR Algorithm

Based on Theorem 2.2 we can develop an implicit double shift quaternion QR algorithm with the help of the JRS-symmetric theory and algorithms.

**Algorithm 4.9 (Implicitly Double Shift Quaternion QR Algorithm).** Given a quaternion matrix \( Q := [Q_0, Q_2, Q_1, Q_3] \), where \( Q_{0,1,2,3} \in \mathbb{H}^{n \times n} \), the following algorithm overwrites \( Q \) with the quasi upper-triangular Schur matrix \( T := [T_0, T_2, T_1, T_3] \) which satisfies \( T = W^*QW \), where \( W := [W_0, W_2, W_1, W_3] \) is a unitary quaternion matrix.

1. Apply Algorithm 4.3 to calculate the Hessenberg form \( \hat{W}^*Q\hat{W} = H := [H_0, H_2, H_1, H_3] \) of the quaternion matrix \( Q \), where \( \hat{W} := [W_0, W_2, W_1, W_3] \) is a unitary quaternion matrix.
2. Utilize Algorithm 4.8 to calculate the quasi upper-triangular Schur canonical form \( \tilde{W}^* H \tilde{W} = T := [T_0, T_2, T_1, T_3] \) of the quaternion Hessenberg matrix \( H \), where \( \tilde{W} := [W_0, W_2, \bar{W}_1, \bar{W}_3] \) is a unitary quaternion matrix.

3. Calculate \( W = \tilde{W}^* W \).

**Remark 4.12.** Bunse-Gerstner, Byers and Mehrmann [1] straightly suggested to replace \( H \) by \( M = H^2 - (\kappa + \bar{\kappa})H + \kappa \bar{\kappa} I \) in the quaternion QR step. The supporting theory is applying two steps of shifted QR iteration applied to the real counterpart \( T_H \), which is JRS-symmetric; see Section 3.4. Since \( \kappa + \bar{\kappa} \) and \( \kappa \bar{\kappa} \) are real, if \((\lambda, x)\) is an eigenpair of \( H \) then \((\lambda^2 - (\kappa + \bar{\kappa})\lambda + \kappa \bar{\kappa}, x)\) is an eigenpair of \( M \).

**Remark 4.13.** The eigenvectors of the original quaternion matrix \( Q \) can be found by computing the eigenvectors of the quasi upper-triangular Schur matrix \( T \) produced by Algorithm 4.9, and transforming them back under the unitary quaternion transformation \( W \). Thus the problem of finding the eigenvectors of the original quaternion matrix \( Q \) is reduced to computing the eigenvectors of a quasi-triangular quaternion matrix \( T \). We will study this project in further.

The main differences between Algorithm 4.9 and Algorithm A5 in [1] are as follows.

1. By Algorithm 4.9, the calculated Hessenberg matrix \( H \) in step 1 has real subdiagonal entries, and this structure is preserved in step 2 (see steps 4-5 in Algorithm 4.8); and hence, the subdiagonal entries of the resulted quasi upper-triangular Schur form are real. The subdiagonal entries of the calculated Hessenberg form by Algorithm A5 in [1] are not necessary to be real.

2. In Algorithm 4.9 the smallest magnitude eigenvalues of the 2-by-2 right-down submatrix of the unreduced Hessenberg quaternion matrix and its conjugate are chosen as the double shifts, while the last diagonal element and its conjugate are chosen in [1, Algorithm A5].

3. The calculation of Algorithm 4.9 is only in real arithmetic, while Algorithm A5 in [1] runs in quaternion operations.

## 5 Numerical experiment

In this section we present four numerical examples to compare the efficiency of newly proposed algorithms with the state-of-the-art algorithms. All numerical experiments are performed on a personal computer with 2.4GHz Intel Core i7 and 8GB 1600 MHz DDR3, and all codes are written in MATLAB using MATLAB version 9.0.0.321247 (2016a).

**Example 5.1 (Upper Hessenberg Reduction of Quaternion Matrices).** Suppose that

\[
M = M_0 + M_1 i + M_2 j + M_3 k := [M_0, M_2, M_1, M_3]
\]

is a Toeplitz quaternion matrix, where \( M_{0,1,2,3} \) are real matrices of order \( n \), generated by the MATLAB order `toeplitz` as

\[
M_0 = \text{toeplitz}(C, R), M_1 = \text{toeplitz}(R), M_2 = \text{toeplitz}(C), M_3 = \text{toeplitz}(R, C),
\]

with \( C = [n, 1 : n, n] \) and \( R = C(n : -1 : 1) \). For \( n=100:100:2000 \), we compare the numerical efficiency of the following algorithms on Hessenberg reduction:
Figure 5.1: The CPU times (seconds) and the relative residuals for quaternion Hessenberg reduction

- **hessq**: Algorithm A3 in [1] based on the quaternion Householder-based transformation([1], Algorithms A2]) and using quaternion toolbox [22];
- **hessQH1**: based on the quaternion Householder-based transformation $\mathcal{H}_1$ in [21];
- **hessQH2**: based on the quaternion Householder-based transformation $\mathcal{H}_2$ or $\mathcal{H}_4$ in [21];
- **hessQH1im**: Algorithm 4.1;
- **hessQH2im**: Algorithm 4.2;
- **hessQH3**: Algorithm 4.3.

In the left figure of Figure 5.1, the CPU times costed by six algorithms are for the calculation of the Hessenberg form $H := [H_0, H_2, H_1, H_3]$ and the unitary matrix $W := [W_0, W_2, W_1, W_3]$.

In the right figure of Figure 5.1, the relative error is defined as

$$Re = \frac{\|\text{tril}(H_0, -2)\|_F + \sum_{s=1}^{3} \|\text{tril}(H_s, -1)\|_F}{\|H_0, H_2, H_1, H_3\|_F}.$$  

Figure 5.1 indicates that

- when the dimension is large, the real structure-preserving algorithms cost less CPU times than the algorithms based on quaternion operations;
- Algorithm 4.1 and Algorithm 4.2 generally are faster than the Hessenberg reduction algorithms based on the Householder-based transformations $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_4$ in [21];
- and the residue of Algorithm 4.3 is generally smaller than those of Algorithm 4.1 and Algorithm 4.2.

**Example 5.2 (QR Decompositions of Quaternion Hessenberg Matrices).** Suppose that

$$H = H_0 + H_1i + H_2j + H_3k := [H_0, H_2, H_1, H_3]$$  

29
is a random upper quaternion Hessenberg matrix with the real counterpart JRS-symmetric, where \( H_{0,1,2,3} \in \mathbb{R}^{n \times n} \). For \( n=100:100:4000 \), we compare the numerical efficiency of the following two quaternion Givens transformations on the QR decomposition of \( H \):

- **FGivensQ**: applying fast Givens transformation in [18];
- **GGivensQ**: Algorithm 4.5.

In the left figure of Figure 5.2, the CPU times costed by two algorithms **FGivensQ** and **GGivensQ** are for the calculation of the upper JRS-triangular matrix \( R := [R_0, R_2, R_1, R_3] \) and the Q factor \( W := [W_0, W_2, W_1, W_3] \). In the right figure of Figure 5.2, the relative residual is defined as

\[
Re = \frac{\|A - WR\|_F}{\|A\|_F}.
\]

From the numerical results in Figure 5.2, we can see that when the dimension is very large **GGivensQ** is faster than **FGivensQ** and the relative residual of **GGivensQ** is smaller.

**Example 5.3 (Hessenberg reduction of \( H_F \)).** Suppose that

\[
H_F = H^F_0 + H^F_1 i + H^F_2 j + H^F_3 k := [H^F_0, H^F_2, H^F_1, H^F_3]
\]

is the broken Hessenberg quaternion matrix in Francis QR step, where \( H^F_{0,1,2,3} \) are \( n \times n \) real matrices as defined in Section 3.4.2. For \( n=4000:100:7000 \), we compare the numerical efficiency of the following algorithms on Hessenberg reduction of \( H_F \): Algorithm 4.1 (\texttt{hessQ1im}), Algorithm 4.2 (\texttt{hessQH2im}), Algorithm 4.3 (\texttt{hessQH3}), the Hessenberg reduction based on fast Givens transformation (\texttt{hessQ-FGivensQ}), and Algorithm 4.4 (\texttt{hessQ-GGivensQ}). In the left figure of Figure 5.3, the CPU times costed by four algorithms are for the calculation of the upper JRS-Hessenberg form \( \hat{H} := [\hat{H}_0, \hat{H}_2, \hat{H}_1, \hat{H}_3] \) and the orthogonally JRS-symplectic matrix \( \hat{W} := [\hat{W}_0, \hat{W}_2, \hat{W}_1, \hat{W}_3] \). In the right figures of Figure 5.3, the backward error is defined as

\[
ERR = \|H_F \hat{W} - \hat{W} \hat{H}\|_F.
\]
Figure 5.3: The CPU times (seconds) and the relative residuals for quaternion Hessenberg reduction.
Example 5.4 (Schur Decompositions of Quaternion Matrices). A newly proposed technique of the copyright protection of color image is the blind watermarking scheme based on Schur decomposition. The features obtained by Schur decomposition are used for embedding watermark and extracting watermark in the blind manner. These watermarking algorithms have a very good performance, such as in the aspects of the invisibility, robustness, computational complexity, security, capacity etc.; see [29] for more details.

We apply Algorithm 4.9 to compute the quasi upper-triangular Schur decompositions of purely imaginary quaternion matrices denoting color images. The color image for testing is the standard Lena image of order $512$, denoted by $M = M_1 i + M_2 j + M_3 k := [0, M_2, M_1, M_3]$, where all elements of $M_{1,2,3} \in \mathbb{R}^{512 \times 512}$ are nonnegative but not bigger than $1$.

Let $n$ denote the order of the principle submatrix of $M$. For $n=12:10:512$, we compare the numerical efficiency of two QR algorithms with different kinds of shift:

- Quaternion QR Algorithm 4.5, Algorithm A5 (QRASq);
- Algorithm 4.9 with the shift suggested in Section 4.4 (QRASQ).

The CPU times reported in Figure 5.4 are for the calculation of the JRS-Schur form $T := [T_0, T_2, T_1, T_3]$ and the orthogonally JRS-symplectic matrix $W$.

6 Conclusion

A structure-preserving QR algorithm is presented to calculate the quasi upper-triangular Schur forms of quaternion matrices. The strategy is to preserve the algebraic symmetry of the real counterpart in the processing and to be in real arithmetic. The storage and cost of the newly proposed algorithm are reduced to the same level of the traditional QR algorithm in quaternion arithmetic with same accuracy and stability. The main contribution of this paper can be concluded as follows.

- Prove that once the first column of each block of the orthogonally JRS-symplectic reduction matrix is decided, the upper JRS-Hessenberg form is unique under the similarity
transformation by a diagonal matrix; propose the Francis $JRS$-QR step and a QR algorithm for computing the real $JRS$-Schur form with preserving the upper $JRS$-Hessenberg structure.

- Define a novel quaternion Givens transformation and apply it to compute the QR decomposition of quaternion Hessenberg matrix; develop a new implicit double shift quaternion QR algorithm which only executes real operations and preserves the structures of quaternion matrices.

- The newly proposes real structure-preserving quaternion QR algorithm only need to store the real part and three imaginary parts and apply real operations on them directly. We are sure that this is a novel method of computing the right eigenvalues of general quaternion matrices.

Numerical examples show that the newly proposed algorithms are fast and reliable, and that the larger the dimension of the problem, the better are they than the state-of-the-art algorithms.

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