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A CORE-CHASING SYMPLECTIC QR ALGORITHM*

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Abstract. A structure preserving QR algorithm is developed for a set of symplectic matrices with a certain rank condition. The algorithm is constructed based on a factorization presentation of a symplectic Hessenberg matrix and core-chasing type QR iterations. It preserves the symplectic structure in the sense that only unitary symplectic matrices are used for similarity transformations. The proposed algorithm is theoretically equivalent to Mehrmann's algorithm. In practice, it is more numerically stable. Two economic versions of the algorithm are also provided that use the symplectic structure more efficiently meanwhile at the risk of losing numerical stability. The same idea applies to the symplectic pairs and a core-chasing symplectic QZ algorithm can be developed.

Key words. symplectic QR algorithm, symplectic matrices, symplectic pairs, symplectic Givens rotations, symplectic Householder matrices, core-chasing

AMS subject classifications. 65F15, 65H10, 93D15

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1. Introduction.

The numerical eigenvalue problem of symplectic matrices and pairs plays a fundamental role in systems and control and other areas, and has been studied for decades, e.g., [4, 13, 17, 18, 21, 22]. A symplectic matrix or pair has nice block structures and its eigenstructure exhibits elegant symmetric patterns. For instance, the eigenvalues of a symplectic matrix are in pairs as $(\lambda, \bar{\lambda}^{-1})$. For numerical efficiency and accuracy, the concept of structure preserving methods has been introduced for such structured matrices and pairs. For the eigenvalue problem of symplectic matrices/pairs, a general idea is to preserve the symplectic structure during the computational process. Based on the fact that similarity transformations with symplectic matrices preserve the symplectic structure, several QR/QZ type structure preserving algorithms have been developed [2, 3, 8, 9, 13, 14, 16, 20, 21]. However, the use of nonunitary symplectic similarity transformations may cause numerical instability problems. So far, the only known QR/QZ algorithm that uses similarity transformations with unitary and symplectic matrices is presented in [20] for the symplectic matrices/pairs with a certain rank condition. There is no such algorithm for general symplectic matrices/pairs due to the lack of appropriate condensed forms for performing QR iterations. For the Hamiltonian matrices/pairs, which are closely related to the symplectic matrices/pairs, the situation is similar, e.g., [5, 6, 7, 10, 11, 12, 15]. However, unlike the Hamiltonian QR algorithm in [10, 11], a structure preserving algorithm like the one in [20] may still not be able to simultaneously achieve both goals of preserving the symplectic structure and maintaining numerical backward stability. This is because in a finite floating point number system, rounding errors make it difficult to preserve the symplectic structure even with transformations that are theoretically structure preserving. In fact, it is already a difficult problem to store a symplectic matrix so that it is exactly symplectic on a computer. The same arguments apply to the so-called symplectic upper Hessenberg form, a condensed form that the algorithm in [20] is based on. One additional problem is that the symplectic upper Hessenberg form is only semi-explicit, i.e., it only exhibits half of the structure

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with a zero pattern while another half hides under the symplectic property. With such a semi-explicit form it is possible that the symplectic structure may deteriorate during an iteration process. This, in turn, causes an algorithm like the one in [20] to potentially lose numerical stability, since the iterations rely on the symplectic upper Hessenberg structure.

In this paper, we present a symplectic QR algorithm for the same type of symplectic matrices considered in [20]. These symplectic matrices have the following additional property: if such a symplectic matrix is partitioned as a 2×2 block matrix with equal block size, its $(2, 1)$ (or $(1, 2)$) block is rank one. Such a symplectic matrix may arise from single input/output control problem. Examples can be found in [4] and the references therein. A symplectic matrix with the above rank condition can be transformed to a symplectic upper Hessenberg matrix with a unitary symplectic similarity transformation. The proposed algorithm follows exactly the same idea given in [20], but uses different techniques. We express a symplectic Hessenberg matrix in a factored form and introduce a direct reduction process for computing such a form. The factored form allows us to implement core-chasing type QR iterations as those in [1, 23, 24]. The factored form exploits additional structures of a standard symplectic upper Hessenberg matrix. This provides the opportunity for finding more efficient ways to preserve the symplectic structure and improve numerical stability. The proposed algorithm takes this advantage. Also, we will show that a core-chasing symplectic QZ algorithm can be developed for symplectic pairs.

The paper is organized as follows. In section 2 we define the symplectic matrices and pairs, and introduce some elementary unitary symplectic matrices used in the algorithms. Some transformations used in the core-chasing symplectic QR iterations will also be introduced. In section 3 we present the proposed symplectic QR algorithm. We provide detailed descriptions of an initial reduction process that transforms a symplectic matrix with the rank one condition to a symplectic upper Hessenberg matrix in a factored form. We describe the implementations of core-chasing symplectic QR iteration both in single and double shift cases. We show two additional versions of the algorithm that take further use of the symplectic upper Hessenberg structure based on the factored form. They are more structure preserving but might be less numerically stable. In this section, the choices of shifts and the deflation criterion are also discussed, and numerical testing results are reported to show the effectiveness of the proposed algorithms and compare them with the algorithm from [20]. In section 4 we generalize to the symplectic pair case and show that a core-chasing symplectic QZ algorithm can be constructed in the same way. Our conclusions are given in section 5.

Throughout the paper, the $n \times n$ identity matrix is denoted by I_n or I, and its ith column is denoted by e_i. The transpose and adjoint (conjugate transpose) of a matrix A are denoted by A^T and A^*, respectively. A matrix $A = [a_{ij}]$ is upper triangular, Hessenberg, and t-Hessenberg if $a_{ij} = 0$ for all $i > j$, $i > j + 1$, and $i > j + 2$, respectively. So an upper t-Hessenberg matrix is an upper Hessenberg matrix plus possibly nonzero entries along the 2nd subdiagonal. Similarly, a matrix is lower triangular, Hessenberg, and t-Hessenberg if its transpose is upper triangular, Hessenberg, and t-Hessenberg, respectively. A matrix in a 2×2 block form

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

with the blocks of equal size is skew upper triangular if $A_{21} = 0$, A_{11} is upper triangular, and A_{22} is lower triangular. Finally, $\|\cdot\|$ is the 2-norm.

2. Preliminaries. Let

$$\mathcal{J}_n = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}.$$

A matrix $\mathcal{S} \in \mathbb{C}^{2n\times 2n}$ is symplectic if $\mathcal{S}\mathcal{J}_n\mathcal{S}^* = \mathcal{J}_n$. Note that if $\mathcal{S}$ is symplectic, $\mathcal{S}^{-1}$, $\mathcal{S}^*$, $\mathcal{S}^{-*}$ are all symplectic as well. Also, a product of symplectic matrices is symplectic. A matrix $\mathcal{S}$ is symplectic upper triangular if

$$\mathcal{S} = \begin{bmatrix} S_{11} & S_{12} \\ 0 & S_{11}^{-*} \end{bmatrix},$$

where S_{11} is upper triangular and $S_{12}S_{11}^* = S_{11}S_{12}^*$, i.e., $S_{12}S_{11}^*$ is Hermitian. So a symplectic upper triangular matrix is both symplectic and skew upper triangular. If S_{11} is not upper triangular, the above matrix is called block symplectic upper triangular. In principle, a block symplectic upper triangular matrix is characterized by a matrix pair (S_{11}, S_{12}) with S_{11} invertible and $S_{11}S_{12}^* = S_{12}S_{11}^*$. A more compact characterization is to use a matrix pair (S_{11}, W), where S_{11} is invertible and $W = W^*$, by considering $S_{12} = WS_{11}^{-*}$. A matrix $\mathcal{S}$ is symplectic upper Hessenberg if

$$\mathcal{S} = \begin{bmatrix} S_{11} & S_{12} \\ se_n^* & S_{22} \end{bmatrix}$$

is symplectic, S_{11} is upper Hessenberg, and $s \in \mathbb{C}^n$ is a column vector. A matrix $\mathcal{V}$ is unitary symplectic if it is both unitary and symplectic. A unitary symplectic matrix has the block form

$$\begin{bmatrix} V_1 & V_2 \\ -V_2 & V_1 \end{bmatrix}$$

with $V_1^*V_1 + V_2^*V_2 = I$ and $V_1^*V_2 = V_2^*V_1$. $\mathcal{V}$ is (real) orthogonal symplectic if it is real and unitary symplectic. Any symplectic matrix $\mathcal{S}$ has a symplectic QR factorization $\mathcal{Q}\mathcal{R}$, where $\mathcal{Q}$ is unitary symplectic and $\mathcal{R}$ is symplectic upper triangular. If a symplectic matrix $\mathcal{S}$ has no unimodular eigenvalues, then there exist a unitary symplectic matrix $\mathcal{Q}$ and a symplectic upper triangular matrix $\mathcal{R}$ such that $\mathcal{S} = \mathcal{Q}\mathcal{R}\mathcal{Q}^*$. This is a symplectic Schur form. If $\mathcal{S}$ has unimodular eigenvalues, then a symplectic Schur form may or may not exist, depending on the properties of the unimodular eigenvalues (see [19]).

A matrix pair $(\mathcal{A}, \mathcal{B})$ with $\mathcal{A}, \mathcal{B} \in \mathbb{C}^{2n\times 2n}$ is symplectic if $\mathcal{A}\mathcal{J}_n\mathcal{A}^* = \mathcal{B}\mathcal{J}_n\mathcal{B}^*$. Note that if one of $\mathcal{B}$ and $\mathcal{A}$ is invertible, then both are invertible and $\mathcal{B}^{-1}\mathcal{A}$ is a symplectic matrix.

An $n \times n$ Householder reflector has an expression

$$H(v) = I_n - 2\frac{vv^*}{v^*v}, \qquad 0 \neq v \in \mathbb{C}^n.$$

By convention, $H(0) = I$. For each $i \in \{1, \ldots, n\}$ the set of the Householder reflectors with $v \in \mathbb{C}^n$ and $v_{i+1} = \cdots = v_n = 0$ is denoted by $\mathbb{H}_i$. A symplectic Householder reflector is a block diagonal matrix

$$\mathcal{H}(v) = \begin{bmatrix} H(v) & 0 \\ 0 & H(v) \end{bmatrix},$$

where $H(v)$ is a Householder reflector. We use $\mathbb{SH}_i$ to denote the sets of $\mathcal{H}(v)$ with $H(v) \in \mathbb{H}_i$.

An $n \times n$ Givens rotation is given by

$$G_{ij}(\alpha,\beta) = \begin{bmatrix} I_{i-1} & & & & \\ & \alpha & & \beta & \\ & & I_{j-i-1} & & \\ & -\bar{\beta} & & \bar{\alpha} & \\ & & & & I_{n-j} \end{bmatrix}, \quad \alpha,\beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1,$$

where $1 \le i < j \le n$. We will not show the scalars α, β if they are not important in the context. The set of the Givens rotations with a given integer pair (i,j) is denoted by $\mathbb{G}_{ij}$. For brevity, we will use the notations $G_i := G_{i,i+1}$ and $\mathbb{G}_i := \mathbb{G}_{i,i+1}$. We will mainly use two types of symplectic Givens rotations. The first type has a form

$$\mathcal{G}_{ij}(\alpha,\beta) = \begin{bmatrix} G_{ij}(\alpha,\beta) & \\ & G_{ij}(\alpha,\beta) \end{bmatrix}, \qquad G_{ij}(\alpha,\beta) \in \mathbb{G}_{ij}.$$

The set of such rotations with a fixed pair (i,j) is denoted by $\mathbb{SG}_{ij}$. Similarly, we will use the notations $\mathcal{G}_i := \mathcal{G}_{i,i+1}$ and $\mathbb{SG}_i := \mathbb{SG}_{i,i+1}$ for $i = 1, \ldots, n-1$. The second type of symplectic Givens rotations has a form

$$\Gamma_i := \Gamma_i(\alpha,\beta) = G_{i,n+i}(\alpha,\beta) \in \mathbb{R}^{2n\times 2n}, \quad \alpha,\beta \in \mathbb{R}, \quad \alpha^2 + \beta^2 = 1, \quad 1 \le i \le n.$$

We will use Γ_n only in the algorithms. The set of all Γ_n is denoted by $\mathbb{SG}_n$. Note for a Givens rotation or a symplectic Givens rotation, its determinant is 1.

The following simple results are fundamental for performing the core-chasing QR iterations, which can be found in [1, 23, 24].

Lemma 2.1. *Any 3×3 unitary matrix U with $\det U = 1$ can be expressed as a product of three Givens rotations in the form*

$$U = G_1(a_1,b_1)G_2(a_2,b_2)G_1(a_3,b_3), \tag{2.1}$$

and in the form

$$U = G_2(c_1,d_1)G_1(c_2,d_2)G_2(c_3,d_3). \tag{2.2}$$

Proof. See [1, sect. 1.4] for the proof. ∎

From the above result, it is obvious that for any $1 \le i \le n-1$, an $n \times n$ unitary matrix in a product form $G_i(a_1,b_1)G_{i+1}(a_2,b_2)G_i(a_3,b_3)$ can be expressed as another product $G_{i+1}(c_1,d_1)G_i(c_2,d_2)G_{i+1}(c_3,d_3)$ and vice versa. Such a transformation in either direction is called a *turnover* (see [1]), and we will use the symbol $(i,i+1,i) \to (i+1,i,i+1)$ or $(i+1,i,i+1) \to (i,i+1,i)$ if necessary. The turnover transformations play a fundamental role in core-chasing. So we will use the same kind of symbols for a composite turnover process. For instance,

$$(\mathbf{4},\mathbf{3},\mathbf{4},2,3,1,2) \to (3,4,\mathbf{3},\mathbf{2},\mathbf{3},1,2) \to (3,4,2,3,\mathbf{2},\mathbf{1},\mathbf{2}) \to (3,4,2,3,1,2,1),$$

means that for the product of seven Givens rotations $G_4G_3G_4G_2G_3G_1G_2$ we perform turnovers first to the product of the first three matrices, then the product from the third to the fifth, and finally the product of the last three. In the above product from the same notations, say the two G_4's in the first tuple, can be different Givens rotations but both in $\mathbb{G}_4$. We will also use the symbols $(\ldots,\mathbf{i},\mathbf{j},\ldots) = (\ldots,\mathbf{j},\mathbf{i},\ldots)$

for the interchange $G_iG_j = G_jG_i$ (when $|i-j| \geq 2$), and $(\ldots, \mathbf{i}, \mathbf{i}, \ldots) = (\ldots, \mathbf{i}, \ldots)$ for expressing a product of two Givens rotations from $\mathbb{G}_i$ as a single one in the same $\mathbb{G}_i$. The same symbols will also be used for a product of symplectic Givens rotations.

The symplectic matrices considered in this paper are the same as those considered in [20]. They are characterized by

$$\mathcal{S} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}, \quad S_{ij} \in \mathbb{C}^{n \times n}, \quad i, j = 1, 2; \quad \operatorname{rank} S_{21} = 1. \tag{2.3}$$

If $\operatorname{rank} S_{12} = 1$ instead, we may turn to consider the matrix $\mathcal{S}^*$ or $\mathcal{S}^T$. These are the only known symplectic matrices that can be transformed to a symplectic upper Hessenberg form with a finite number of unitary symplectic similarity transformations. In [20] a symplectic QR algorithm is presented for solving the eigenvalue problem of such a symplectic matrix. See Algorithm 1.

Algorithm 1 [Symplectic QR Algorithm] (see [20])

1. Determine a unitary symplectic matrix $\mathcal{V}_0$ such that $\tilde{\mathcal{S}} := \mathcal{V}_0^* \mathcal{S} \mathcal{V}_0$ is symplectic upper Hessenberg.
2. Perform the following QR iteration until $\tilde{\mathcal{S}}$ converges:
   (a) Update $\tilde{\mathcal{S}} := \mathcal{Y}^* \tilde{\mathcal{S}} \mathcal{Y}$ with a block diagonal unitary symplectic matrix
   $$\mathcal{Y} = \begin{bmatrix} Y & 0 \\ 0 & Y \end{bmatrix}.$$
   (b) Update $\tilde{\mathcal{S}} := \mathcal{X}^* \tilde{\mathcal{S}} \mathcal{X}$ with a unitary symplectic matrix in a product form with at least one or two factors from $\mathbb{SG}_n$.
   (c) Update $\tilde{\mathcal{S}} := \mathcal{Z}^* \tilde{\mathcal{S}} \mathcal{Z}$ with another block diagonal unitary symplectic matrix
   $$\mathcal{Z} = \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix}.$$

In each symplectic QR iteration, the unitary symplectic matrix $\mathcal{Q} := \mathcal{Y}\mathcal{X}\mathcal{Z}$ is the Q factor of a symplectic QR factorization of the symplectic matrix $(\tilde{\mathcal{S}} - \sigma I)^{-1}(\bar{\sigma}\tilde{\mathcal{S}} - I)$ in the single shift case, or $(\tilde{\mathcal{S}}^2 - \mu\tilde{\mathcal{S}} + \nu I)^{-1}(\nu\tilde{\mathcal{S}}^2 - \mu\tilde{\mathcal{S}} + I)$ in the double shift case.

3. Core-chasing symplectic QR algorithm.

In this section we will provide a different version of Algorithm 2. We will follow the same steps, but use different techniques based on different interpretations. The main changes include a factored form of a symplectic Hessenberg matrix and core-chasing symplectic QR iterations. The detailed descriptions of these changes are provided below. For completeness we will also briefly discuss the choices of shifts and deflation criterion.

3.1. Symplectic upper Hessenberg form reduction.

In [20], a reduction procedure is provided for computing a unitary symplectic matrix $\mathcal{V}_0$ and a symplectic upper Hessenberg matrix $\tilde{\mathcal{S}}$ satisfying

$$\mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 = \begin{bmatrix} \tilde{S}_{11} & \tilde{S}_{12} \\ s e_n^* & \tilde{S}_{22} \end{bmatrix} = \tilde{\mathcal{S}}$$

for a given symplectic matrix $\mathcal{S} \in \mathbb{C}^{2n \times 2n}$ satisfying (2.3), where $\tilde{S}_{11}$ is upper Hessenberg and $s \in \mathbb{C}^n$. Since $\tilde{S}_{11}$ is upper Hessenberg, there exist an upper triangular matrix T_{11} and a unitary matrix $G = G_1 \dots G_{n-1}$ with $G_i \in \mathbb{G}_i$ for $i = 1, \dots, n-1$, such that $\tilde{S}_{11} = GT_{11}$. This is a QR factorization of $\tilde{S}_{11}$, which can be obtained by premultiplying $G_1^*, \dots, G_{n-1}^*$, respectively, to annihilate the subdiagonal entries of $\tilde{S}_{11}$ in the order $(2,1), \dots, (n, n-1)$. Define

$$\mathcal{G} = \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix}.$$

The $(1,1)$ block of $\mathcal{G}^* \tilde{\mathcal{S}}$ is T_{11}, and following the symplectic property the $(2,1)$ block is a scalar multiple of $e_n e_n^*$. One can show there is $\Gamma_n \in \mathbb{SG}_n$ so that $\Gamma_n^T \mathcal{G}^* \tilde{\mathcal{S}} = \mathcal{T}$ is symplectic upper triangular. Then $\tilde{\mathcal{S}} = \mathcal{G} \Gamma_n \mathcal{T}$. Note $\mathcal{G} = \mathcal{G}_1 \dots \mathcal{G}_{n-1}$ for

$$\mathcal{G}_i = \begin{bmatrix} G_i & 0 \\ 0 & G_i \end{bmatrix},$$

$i = 1, \dots, n-1$. By redefining $\mathcal{V}_0 := \mathcal{V}_0 \mathcal{G} \Gamma_n$, we have

$$\tilde{\mathcal{S}} := \mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 = \mathcal{T} \mathcal{G} \Gamma_n, \quad \mathcal{T} = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{11}^{-*} \end{bmatrix}, \quad \mathcal{G} = \mathcal{G}_1 \dots \mathcal{G}_{n-1} = \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix}, \tag{3.1}$$

with $T_{12} T_{11}^* = T_{11} T_{12}^*$, and $\tilde{\mathcal{S}}$ is still symplectic upper Hessenberg. This is the factored form that will be used in the core-chasing symplectic QR iterations. The factored form shows that a symplectic upper Hessenberg form can be characterized by unitary matrices G and Γ_n and a matrix pair (T_{11}, T_{12}) defined in (3.1). It exploits the hidden structures of a symplectic upper Hessenberg matrix. Recall that the matrix pair (T_{11}, T_{22}) can be replaced by a more compact version (T_{11}, W) with a Hermitian W satisfying $W = T_{12} T_{11}^*$.

We now introduce a direct reduction procedure for computing (3.1). For a symplectic matrix in the form (2.3), S_{21} can be expressed as

$$S_{21} = b f g^*, \quad \|f\| = \|g\| = 1, \quad b \neq 0.$$

Due to the symplectic structure one has

$$b S_{11}^* f g^* = \bar{b} g f^* S_{11}, \quad \bar{b} S_{22} g f^* = b f g^* S_{22}^*.$$

This implies that

$$S_{11}^* f = (f^* S_{11} g) \frac{\bar{b}}{b} g, \quad S_{22} g = (g^* S_{22}^* f) \frac{b}{\bar{b}} f. \tag{3.2}$$

Let $H_n, \tilde{H}_n \in \mathbb{H}_n$ be Householder reflectors such that $H_n^* g = \rho e_n$ and $\tilde{H}_n^* f = \tilde{\rho} e_n$ with $|\rho| = |\tilde{\rho}| = 1$. Define

$$\mathcal{H}_n = \begin{bmatrix} H_n & 0 \\ 0 & H_n \end{bmatrix} \quad \text{and} \quad \tilde{\mathcal{H}}_n = \begin{bmatrix} \tilde{H}_n & 0 \\ 0 & \tilde{H}_n \end{bmatrix}.$$

By using the symplectic structure, one has

$$\tilde{\mathcal{H}}_n^* \mathcal{S} \mathcal{H}_n = \begin{bmatrix} \tilde{H}_n^* S_{11} H_n & \tilde{H}_n^* S_{12} H_n \\ b e_n e_n^* & \tilde{H}_n^* S_{22} H_n \end{bmatrix}, \quad b := \bar{\rho} \tilde{\rho} b,$$

and similar to (3.2),

$$(\tilde{H}_n^* S_{11} H_n)^* e_n = \frac{c\bar{b}}{b} e_n, \quad c := e_n^* (\tilde{H}_n^* S_{11} H_n) e_n, \tag{3.3}$$

$$(\tilde{H}_n^* S_{22} H_n) e_n = \frac{\bar{a}b}{\bar{b}} e_n, \quad a := e_n^* (\tilde{H}_n^* S_{22} H_n) e_n. \tag{3.4}$$

By comparing the last component on both sides of (3.4), one has $a\bar{b} = \bar{a}b$, i.e., $a\bar{b}$ is real. Since $b \neq 0$, a matrix $\Gamma_n = \Gamma_n(\phi, \psi) \in \mathbb{SG}_n$ can be constructed with

$$\phi = \frac{a\bar{b}}{|b|\sqrt{|a|^2 + |b|^2}}, \quad \psi = -\frac{|b|}{\sqrt{|a|^2 + |b|^2}},$$

so that

$$\tilde{\mathcal{H}}_n^* \mathcal{S} \mathcal{H}_n \Gamma_n^T = \begin{bmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ 0 & \tilde{T}_{11}^{-*} \end{bmatrix},$$

which is block symplectic upper triangular. Because $\tilde{\mathcal{H}}_n$ and $\mathcal{H}_n$ are block diagonal, one has

$$\mathcal{H}_n^* \mathcal{S} \mathcal{H}_n \Gamma_n^T = \mathcal{H}_n^* \tilde{\mathcal{H}}_n \begin{bmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ 0 & \tilde{T}_{11}^{-*} \end{bmatrix} =: \begin{bmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ 0 & \tilde{T}_{11}^{-*} \end{bmatrix} =: \tilde{\mathcal{T}}. \tag{3.5}$$

Note that the Householder reflector $\tilde{H}_n$ is used just for determining a, the last component of the vector $\tilde{H}_n^* S_{22} H_n e_n$. It is not involved in the transformations.

The rest of the procedure is just to transform $\tilde{T}_{11}$ in (3.5) to an upper triangular matrix by using a sequence of elementary unitary matrices to annihilate the nonzero entries in the strictly lower triangular part from row n to row 2. We first determine a Householder reflector $H_{n-1} \in \mathbb{H}_{n-1}$ such that the first $n-2$ entries on row n of $\tilde{T}_{11} H_{n-1}$ become zero. We then determine a Givens rotation $G_{n-1} \in \mathbb{G}_{n-1}$ such that the $(n-1, n)$ entry of $\tilde{T}_{11} H_{n-1} G_{n-1}^*$ is zero. Let

$$\mathcal{H}_{n-1} = \begin{bmatrix} H_{n-1} & 0 \\ 0 & H_{n-1} \end{bmatrix}$$

and

$$\mathcal{G}_{n-1} = \begin{bmatrix} G_{n-1} & 0 \\ 0 & G_{n-1} \end{bmatrix}.$$

Then $\mathcal{H}_{n-1}^* \mathcal{H}_n^* \mathcal{S} \mathcal{H}_n \Gamma^T \mathcal{H}_{n-1} \mathcal{G}_{n-1}^*$ is still block symplectic upper triangular but the last row of its $(1,1)$ block is zero but the entry (n,n). Continuing this process, we eventually have the symplectic Householder reflectors $\mathcal{H}_i \in \mathbb{SH}_i$ for $i = 2, \ldots, n$, and the symplectic Givens rotations $\mathcal{G}_i \in \mathbb{SG}_i$, for $i = 1, \ldots, n-1$, such that

$$\mathcal{H}_2^* \ldots \mathcal{H}_{n-2}^* \mathcal{H}_{n-1}^* \mathcal{H}_n^* \mathcal{S} \mathcal{H}_n \Gamma_n^T \mathcal{H}_{n-1} \mathcal{G}_{n-1}^* \mathcal{H}_{n-2} \mathcal{G}_{n-2}^* \ldots \mathcal{H}_2 \mathcal{G}_2^* \mathcal{G}_1^* = \mathcal{T}$$

is symplectic upper triangular. Observe that $\mathcal{G}_i^*$ commutes with $\mathcal{H}_j$ for all $j < i$ and Γ_n^T commutes with $\mathcal{H}_j$ for all $j < n$. Therefore, for

$$\mathcal{V}_0 = \mathcal{H}_n \mathcal{H}_{n-1} \ldots \mathcal{H}_2, \quad \mathcal{G} = \mathcal{G}_1 \mathcal{G}_2 \ldots \mathcal{G}_{n-1},$$

one has $\mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 = \mathcal{T} \mathcal{G} \Gamma_n$, which is (3.1).

Note that a block triangular form (3.5) can be obtained by computing a transformation $\tilde{\Gamma}^T \tilde{\mathcal{H}}_n^* \mathcal{S} \tilde{\mathcal{H}}_n$ with a $\tilde{\Gamma} \in \mathbb{SG}_n$ determined by c and b in (3.3). Note also that the process of transforming $\tilde{T}_{11}$ to an upper triangular matrix is equivalent to that of transforming $\tilde{T}_{22} := \tilde{T}_{11}^{-*}$ to a lower triangular matrix but from column n to column 2. So in the first step one can determine H_{n-1} and G_{n-1} so that either the last row of $H_{n-1}^*\tilde{T}_{11}H_{n-1}G_{n-1}^*$ is parallel to e_n^* or the last column of $G_{n-1}^*H_{n-1}^*\tilde{T}_{22}H_{n-1}$ is parallel to e_n. Let $\tilde{n}_1$ be the 2-norm of the last row of $\tilde{T}_{11}$, and let $\tilde{n}_2$ be the 2-norm of the last column of $\tilde{T}_{22}$. In practice, if $\|\tilde{T}_{22}\|/\tilde{n}_1 < \|\tilde{T}_{11}\|/\tilde{n}_2$, we use the former transformation. Otherwise, we use the latter. Here the matrix 2-norm may be replaced by 1-norm or ∞-norm for saving the computational cost. This strategy is important for numerical stability. The transformation (3.5) is backward stable and the computed $\tilde{\mathcal{T}}$ can be expressed as

$$\begin{bmatrix} \tilde{T}_{11}+\tilde{E}_{11} & \tilde{T}_{12}+\tilde{E}_{12} \\ 0 & \tilde{T}_{11}^{-*}+\tilde{E}_{22} \end{bmatrix} = \mathcal{H}_n^*(\mathcal{S}+\tilde{\mathcal{E}})\mathcal{H}_n\Gamma_n^T = \tilde{\mathcal{T}} + \mathcal{H}_n^*\tilde{\mathcal{E}}\mathcal{H}_n\Gamma_n^T, \tag{3.6}$$

and $\|\tilde{\mathcal{E}}\|, \|\tilde{E}_{11}\|, \|\tilde{E}_{12}\|, \|\tilde{E}_{22}\| = O(\|\mathcal{S}\|_2\mathbf{u})$, where $\mathbf{u}$ is the machine precision, and $\mathcal{H}_n$, Γ_n, $\tilde{\mathcal{T}}$ are the matrices in exact arithmetic. The computed $\tilde{\mathcal{T}}$ is not expected to be exactly symplectic because of the rounding errors. It is close to a symplectic matrix ($\tilde{\mathcal{T}}$) within a distance of order $O(\|\mathcal{S}\|_2\mathbf{u})$. In fact, even $\mathcal{S}$ may be no longer exactly symplectic when it is stored in a finite floating point number system. Nonetheless, we will still call such a transformation structure preserving as long as the matrices involved in the transformation are symplectic. Consider the first transformation performed on $\tilde{T}_{11}+\tilde{E}_{11}$ so that

$$(e_n^*\tilde{T}_{11}+\epsilon_1^*)H_{n-1}G_{n-1}^* = \hat{n}_1 e_n^*, \quad \|\epsilon_1\| = O(\|\mathcal{S}\|\mathbf{u}), \quad |\hat{n}_1| = \tilde{n}_1 + O(\|\mathcal{S}\|\mathbf{u}).$$

Then using $\tilde{T}_{22} = \tilde{T}_{11}^{-*}$, one can show that the last column of the computed $(\tilde{T}_{22}+\tilde{E}_{22})H_{n-1}G_{n-1}^*$ would be $e_n/\bar{\hat{n}}_1+\epsilon_2$ with $\|\epsilon_2\| = O\big(\max\{1, \frac{\|\tilde{T}_{22}\|}{\tilde{n}_1}\}\|\mathcal{S}\|\mathbf{u}\big)$. In the reduction procedure we treat ϵ_2 as zero. Note that the premultiplication of H_{n-1}^* will not affect the above error analysis. When $\|\tilde{T}_{22}\|/\tilde{n}_1$ is large, setting $\epsilon_2 = 0$ may introduce an error of order larger than $O(\|\mathcal{S}\|\mathbf{u})$. So, in general, the above reduction process may not be numerically backward stable. Similarly, the second transformation may introduce errors in the $(1,1)$ block with an order of $O\big(\max\{1, \frac{\|\tilde{T}_{11}\|}{\tilde{n}_2}\}\|\mathcal{S}\|\mathbf{u}\big)$. The above strategy is trying to reduce the order of errors, although it cannot make the method backward stable. Note that the initial symplectic upper Hessenberg form reduction in [20] has a similar numerical stability problem, which could be worse since the above mentioned strategy does not apply. The same strategy can be applied to each and every step in the triangularization process. When these strategies are implemented (including the one for determining $\tilde{H}_n$ and $\tilde{\Gamma}_n$), the resulting factored form will be more general than (3.1) with $\mathcal{G}_1, \dots, \mathcal{G}_{n-1}$ and Γ_n appearing on both sides of $\mathcal{T}$. In order to stay focused on the discussion of the main idea of the algorithm, we will no longer consider this general factored form. We just point out that such a form can be transformed to (3.1) with a finite number of transformations. Also, a core-chasing QR iteration can be constructed directly based on such a general factored form, as in the standard case [1, 24].

The proposed symplectic upper Hessenberg form reduction process requires about $\frac{32}{3}n^3$ flops, while the procedure in [20] requires about $\frac{34}{3}n^3$ flops. If $\mathcal{V}_0$ needs to be formed explicitly, both methods require additional $\frac{4}{3}n^3$ flops.

Note that an economic way for computing (3.1) is to compute the blocks T_{11} and T_{12} only for $\mathcal{T}$ after (3.5) and treat the $(2,2)$ block of $\mathcal{T}$ as T_{11}^{-*}. On the other hand, replacing $\tilde{T}_{11}^{-*}+\tilde{E}_{22}$ in the computed $\tilde{T}$ in (3.6) by $(\tilde{T}_{11}+\tilde{E}_{11})^{-*}$ results in an error in the (2,2) block of order $O(\|\tilde{T}_{11}^{-1}\|^2\|\mathcal{S}\|\mathbf{u})$.

An even more economic way is to compute the pair (T_{11}, W) with $W = W^*$ for $\mathcal{T}$, where $W = T_{12}T_{11}^*$. The Hermitian block W can be computed in the following way. After (3.5), we may compute $\tilde{W} := \tilde{T}_{12}\tilde{T}_{11}^*$. Then $W = H_2^* \dots H_n^* \tilde{W} H_n \dots H_2$. However, $\|\tilde{W}\|$ can be as big as $\|\tilde{T}_{12}\|\|\tilde{T}_{11}\|$. In the worst situation it has an order $O(\|\mathcal{S}\|^2)$. So computing W may introduce an error of order $O(\|\mathcal{S}\|^2\mathbf{u})$.

On the other hand, the two economic procedures reduce the cost from $\frac{32}{3}n^3$ flops to $\frac{23}{3}n^3$ flops and $\frac{19}{3}n^3$ flops, respectively.

In the following subsections we provide two types of core-chasing symplectic QR iterations, the single shift iteration and the double shift iteration, on the full factored form (3.1). We will also discuss how the iterations can be adapted to the two economic cases. For convenience we assume that $\mathcal{S}$ is already in the factored form (3.1).

3.2. Core-chasing symplectic QR iteration: Single shift case. The single shift iteration constructed in [20] uses the fact that for a given shift (scalar) σ and a symplectic matrix $\mathcal{S}$, the matrix $(\mathcal{S} - \sigma I)^{-1}(\bar{\sigma}\mathcal{S} - I)$ is also symplectic. This matrix has a symplectic QR factorization $\mathcal{QR}$, where $\mathcal{Q}$ is unitary symplectic and $\mathcal{R}$ is symplectic upper triangular. A symplectic QR iteration is then carried out by generating another symplectic matrix $\mathcal{Q}^*\mathcal{S}\mathcal{Q}$. When $\mathcal{S}$ is already symplectic upper Hessenberg, so is $\mathcal{Q}^*\mathcal{S}\mathcal{Q}$. The matrix $\mathcal{Q}$ can be expressed as a product of three unitary symplectic matrices,

$$\mathcal{Q} = \mathcal{Y}\Delta\mathcal{Z}, \quad \mathcal{Y} = \begin{bmatrix} Y & 0 \\ 0 & Y \end{bmatrix}, \quad \mathcal{Z} = \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix},$$

where $Y = Y_1 \dots Y_{n-1}$, $Z = Z_{n-1} \dots Z_1$ with $Y_i, Z_i \in \mathbb{G}_i$ $i = 1, \dots, n-1$, and $\Delta = \Gamma_n(\xi, \eta) \in \mathbb{SG}_n$ with $\eta \neq 0$.

In fact, Y is the Q factor of a QR factorization of $\bar{\sigma}S_{11} - I_n$, the (1,1) block of $\bar{\sigma}\mathcal{S} - I$. So the transformation $\mathcal{Y}^*\mathcal{S}\mathcal{Y}$ can be carried out essentially by performing a QR iteration on S_{11}. Assume that $\mathcal{S}$ is already in the factored form (3.1). The matrix $T_{11}G$ and S_{11} are identical except for the last column. Then Y is also the Q factor of a QR factorization of $\bar{\sigma}T_{11}G - I_n$. Therefore, Y can be determined by performing a standard core-chasing QR iteration on $T_{11}G$ with the shift $1/\bar{\sigma}$ [1, 23, 24]. The process can be described as follows. After having determined the Givens rotation $Y_1 \in \mathbb{G}_1$ so that

$$Y_1^*(\bar{\sigma}T_{11}G - I_n)e_1 = Y_1^*(\bar{\sigma}T_{11}G_1e_1 - e_1) \in \operatorname{span}\{e_1\},$$

perform the similarity transformation $Y_1^*T_{11}GY_1$. The matrix $Y_1^*T_{11}$ is upper triangular plus a nonzero $(2,1)$ entry. So there is a Givens rotation $\tilde{Y}_1 \in \mathbb{G}_1$ such that $T_{11} := Y_1^*T_{11}\tilde{Y}_1^*$ is again upper triangular. Recall $G = G_1 \dots G_{n-1}$ with $G_i \in \mathbb{G}_i$ for $i = 1, \dots, n-1$. Hence

$$Y_1^*T_{11}GY_1 =: T_{11}\tilde{Y}_1G_1G_2Y_1G_3 \dots G_{n-1}.$$

Note $\tilde{Y}_1G_1 \in \mathbb{G}_1$. So with a turnover $(\mathbf{1}, \mathbf{2}, \mathbf{1}) \to (2, 1, 2)$, the product $\tilde{Y}_1G_1G_2Y_1$ can be expressed as $\tilde{Y}_2\hat{G}_1\hat{G}_2$ with $\hat{G}_1 \in \mathbb{G}_1$ and $\tilde{Y}_2, \hat{G}_2 \in \mathbb{G}_2$. In the following, for notational simplicity we will make some mild abuse of notation by changing $\hat{G}_1, \hat{G}_2$ to G_1, G_2, respectively. We then have

$$Y_1^*T_{11}GY_1 =: T_{11}\tilde{Y}_2G_1G_2G_3 \dots G_{n-1}.$$

Similarly, there is $Y_2 \in \mathbb{G}_2$ such that $T_{11} := Y_2^*T_{11}\tilde{Y}_2$ is upper triangular. Then

$$Y_2^*Y_1^*T_{11}GY_1Y_2 =: T_{11}G_1G_2G_3G_4 \dots G_{n-1}Y_2 = T_{11}G_1G_2G_3Y_2G_4 \dots G_{n-1}.$$

The product $G_2G_3Y_2$ can be expressed as $\tilde{Y}_3G_2G_3$ with $G_2 \in \mathbb{G}_2$ and $\tilde{Y}_3, G_3 \in \mathbb{G}_3$. So

$$Y_2^*Y_1^*T_{11}GY_1Y_2 =: T_{11}G_1\tilde{Y}_3G_2G_3G_4\dots G_{n-1} = T_{11}\tilde{Y}_3G_1G_2G_3G_4\dots G_{n-1}.$$

The core-chasing process continues until the situation

$$Y^*T_{11}GY =: T_{11}G_1\dots G_{n-1}Y_{n-1}, \quad Y = Y_1Y_2\dots Y_{n-1}, \quad Y_i \in \mathbb{G}_i.$$

Because $G_{n-1}Y_{n-1}$ can be expressed as a single Givens rotation in $\mathbb{G}_{n-1}$, the product form $T_{11}G_1\dots G_{n-2}G_{n-1}Y_{n-1}$ is recovered and a core-chasing QR iteration on $T_{11}G$ is completed. Let

$$\mathcal{Y}_i = \begin{bmatrix} Y_i & 0 \\ 0 & Y_i \end{bmatrix}, \quad \mathcal{G}_i = \begin{bmatrix} G_i & 0 \\ 0 & G_i \end{bmatrix} \in \mathbb{SG}_i, \quad i = 1,\dots,n-1,$$

and

$$\mathcal{Y} = \mathcal{Y}_1\dots\mathcal{Y}_{n-1}, \quad \mathcal{G} = \mathcal{G}_1\dots\mathcal{G}_{n-1},$$

where G_i are the updated Givens rotations. Then

$$\mathcal{Y}^*\mathcal{S}\mathcal{Y} = \mathcal{T}\mathcal{G}\Gamma_n\mathcal{Y}_{n-1}, \tag{3.7}$$

where $\mathcal{T}$ is the updated symplectic upper triangular matrix. The block T_{11} is updated as described above. The $(1,2)$ and $(2,2)$ blocks T_{12} and T_{22} are updated with the same transformations applied to T_{11}. Note T_{22} is not necessarily T_{11}^{-*} in practice, but it is forced to be lower triangular. In exact arithmetic ($T_{22} = T_{11}^{-*}$) the ith transformation $T_{11} := Y_iT_{11}\tilde{Y}_i$ implies that $T_{22} := Y_iT_{22}\tilde{Y}_i$ restores the lower triangular form. Let the 2×2 submatrix of $T_{11}\tilde{Y}_i$ from the $i, i+1$ rows and columns be

$$[a_1, a_2] = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}.$$

Then the 2×2 submatrix of $T_{22}\tilde{Y}_i$ from the same position is

$$[b_1, b_2] = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^{-*} = \bar{d}^{-1}\begin{bmatrix} \bar{a}_{22} & -\bar{a}_{21} \\ -\bar{a}_{12} & \bar{a}_{11} \end{bmatrix},$$

where $d = a_{11}a_{22} - a_{12}a_{21}$. Obviously, the 2×2 Givens rotation in Y_i is for annihilating a_{21} and b_{12} simultaneously. In practice, we use one of the vectors a_1 and b_2 to determine Y_i, depending on which one has a larger norm. With the presence of rounding errors, these two vectors will be $a_1 + \delta_1$ and $b_2 + \delta_2$. Assume $|d| \geq 1$ (or, equivalently, $\|a_1\| > \|b_2\|$) and $\|\delta_1\|$ and $\|\delta_2\|$ are of the same order. In this case we use $a_1 + \delta_1$ to determine the Givens rotation and transform $a_1 + \delta_1$ to ce_1. We then apply the same rotation to $b_2 + \delta_2$ as well. One can show that $b_2 + \delta_2$ is transformed to a vector as $\bar{c}^{-1}e_2 + \delta_3$, where $\|\delta_3\|$ has the same order as $\|\delta_2\|$. If $|d| < 1$, we use $b_2 + \delta_2$ to determine the Givens rotation instead. In this way, enforcing the triangular forms along the iteration process will not increase error order. The same strategy may be adopted for determining $\tilde{Y}_1$ in the initial step.

If we use either the pair (T_{11}, T_{12}) or (T_{11}, W) to represent $\mathcal{T}$, we have the corresponding economic versions of the iteration. In the former case, the iteration is exactly the same except that T_{22} is not updated. The latter case is the same. The only difference is that the Hermitian matrix W is updated with $W := Y_i^*WY_i$, for

$i = 1, \ldots, n-1$. We need to point out in both cases $\tilde{Y}_1$ and $Y_2, \ldots, Y_{n-1}$ are determined by T_{11} only. This potentially makes the iteration less numerically stable.

Back to (3.7), note Γ_n and $\mathcal{Y}_{n-1}$ do not commute. The matrix $\mathcal{Y}^*\mathcal{S}\mathcal{Y}$ is not in the factored form (3.1), nor in a symplectic upper Hessenberg form. In fact, although the $(1,1)$ block of this matrix is again upper Hessenberg, the last two columns of the $(2,1)$ block are nonzero.

The transformation with the symplectic Givens rotation $\Delta = \Gamma_n(\xi, \eta) \in \mathbb{SG}_n$ (other than I) from $\mathcal{Q}$ is to enforce the (2,1) block of $\Delta^T\mathcal{Y}^*\mathcal{S}\mathcal{Y}\Delta$ being rank-one. Let the (n,n) entries of T_{11}, T_{12}, and T_{22} from $\mathcal{T}$ in (3.7) be t_{nn}, $t_{n,2n}$, and $t_{2n,2n}$, respectively. In exact arithmetic, the symplectic property implies that $t_{2n,2n} = 1/\bar{t}_{nn}$ and $t_{n,2n}\bar{t}_{nn}$ is real. In practice, due to the presence of errors we may have

$$t_{nn} = x_1 e^{i\theta_1}, \quad t_{2n,2n} = x_2 e^{i\theta_2}, \quad t_{n,2n} = x_3 e^{i\theta_3},$$

where x_i and θ_i $(i = 1, 2, 3)$ are all real and $x_1 x_2 \approx 1$, $\theta_1 \approx \theta_2 \approx \theta_3$. Note that ξ, η in Δ are real. In order to determine Δ reliably we first replace t_{nn}, $t_{n,2n}$, $t_{2n,2n}$ by $ce^{i\theta}, de^{i\theta}, c^{-1}e^{i\theta}$, respectively, where c, d and θ are determined by minimizing

$$|x_1 e^{i\theta_1} - ce^{i\theta}|^2 + |x_2 e^{i\theta_2} - c^{-1}e^{i\theta}|^2 + |x_3 e^{i\theta_3} - de^{i\theta}|^2.$$

In practice, we use an approximate solution given by

$$c = \begin{cases} \frac{x_1^4+1}{x_1^3+x_2} & |x_1| \geq |x_2|, \\ \frac{x_2^3+x_1}{x_2^4+1} & |x_1| < |x_2|, \end{cases} \qquad d = x_3,$$

$$\tan\theta = \frac{(x_1 c)\sin\theta_1 + (x_2/c)\sin\theta_2 + (x_3 d)\sin\theta_3}{(x_1 c)\cos\theta_1 + (x_2/c)\cos\theta_2 + (x_3 d)\cos\theta_3}.$$

This replacement will not increase the error order if $\theta_1, \theta_2, \theta_3$ are sufficiently close and $x_1 x_2$ is sufficiently close to 1. The replacement is simpler in the matrix pair representation cases. In the first case we simply set $t_{2n,2n} = 1/\bar{t}_{nn}$, i.e., we set $x_2 = 1/x_1$ and $\theta_2 = \theta_1$ in the formulas for c and $\tan\theta$. In the second case, we again set $t_{2n,2n} = 1/\bar{t}_{nn}$. Since W is Hermitian, its (n,n) entry, denoted by w_{nn}, is real. Since $t_{n,2n} = w_{nn}/\bar{t}_{nn}$, for $t_{nn} = x_1 e^{\theta_1}$ we simply have $c = x_1$, $d = w_{nn}/x_1$, and $\theta = \theta_1$. So the replacement is no longer needed.

Assume $t_{nn} = ce^{i\theta}$, $t_{n,2n} = de^{i\theta}$, $t_{2n,2n} = c^{-1}e^{i\theta}$ after the above replacement. One can verify that for $\tilde{\Delta} = \Gamma_n(\tilde{\xi}, \tilde{\eta}) \in \mathbb{SG}_n$ with

$$\tilde{\xi} = \frac{c^{-1}\xi + d\eta}{r}, \quad \tilde{\eta} = \frac{c\eta}{r}, \quad r = \sqrt{(c^{-1}\xi + d\eta)^2 + c^2\eta^2}, \tag{3.8}$$

the matrix $\mathcal{T} := \Delta^T\mathcal{T}\tilde{\Delta}$ is again symplectic upper triangular. Now

$$\Delta^T\mathcal{Y}^*\mathcal{S}\mathcal{Y}\Delta =: \mathcal{T}\mathcal{G}_1 \ldots \mathcal{G}_{n-2}\tilde{\Delta}^T\mathcal{G}_{n-1}\Gamma_n\mathcal{Y}_{n-1}\Delta.$$

From the block structures one needs to determine Δ (and $\tilde{\Delta}$) such that the $(2,1)$ block of $\tilde{\Delta}^T\mathcal{G}_{n-1}\Gamma_n\mathcal{Y}_{n-1}\Delta$ is rank one. This $(2,1)$ block is zero except the 2×2 trailing principal submatrix. So by enforcing the determinant of this submatrix to be zero, and using $\mathcal{G}_{n-1} = \mathcal{G}_{n-1}(\alpha_{n-1}, \beta_{n-1})$, $\mathcal{Y}_{n-1} = \mathcal{G}_{n-1}(a_{n-1}, b_{n-1})$, and $\Gamma_n = \Gamma_n(\phi, \psi)$, the two parameters ξ and η have to satisfy

$$\frac{\xi}{\eta} = \frac{c((|\alpha_{n-1}b_{n-1}|^2 + |\beta_{n-1}a_{n-1}|^2)\phi + 2\mathrm{Re}(\alpha_{n-1}\bar{\beta}_{n-1}a_{n-1}b_{n-1})) - d|b_{n-1}|^2\psi}{(c^{-1}|b_{n-1}|^2 - c|\beta_{n-1}|^2)\psi},$$

where $\mathrm{Re}(a)$ is the real part of a complex number a. In order to avoid possible cancellations when both b_{n-1} and β_{n-1} are small, we may rewrite the above formula by dividing both the numerator and denominator with either $|b_{n-1}|^2$ or $|\beta_{n-1}|^2$, depending on which one is bigger.

Once Δ is determined, we have $\tilde{\Delta}$ with (3.8), and matrix $\mathcal{T}$ can be updated with the formula $\mathcal{T} := \Delta^T \mathcal{T} \tilde{\Delta}$.

For the economic versions, the blocks can be updated in the following ways. In the first case, partition the blocks T_{11} and T_{12} from the old $\mathcal{T}$ as

$$T_{11} := \begin{bmatrix} T_1 & t_1 \\ 0 & ce^{i\theta} \end{bmatrix}, \quad T_{12} := \begin{bmatrix} T_2 & t_2 \\ t_3^* & de^{i\theta} \end{bmatrix},$$

and the $(2,2)$ block is considered as

$$T_{11}^{-*} = \begin{bmatrix} T_1^{-*} & 0 \\ -c^{-1}e^{i\theta} t_1^* T_1^{-*} & c^{-1}e^{i\theta} \end{bmatrix}.$$

The updated blocks are

$$T_{11} := \begin{bmatrix} T_1 & \tilde{t}_1 \\ 0 & r^{-1}e^{i\theta} \end{bmatrix}, \quad T_{12} := \begin{bmatrix} T_2 & \tilde{t}_2 \\ \tilde{t}_3^* & \tilde{d}e^{i\theta} \end{bmatrix},$$

where r, $\tilde{\xi}$, $\tilde{\eta}$ are given in (3.8),

$$[\tilde{t}_1, \tilde{t}_2] = [t_1, t_2] \begin{bmatrix} \tilde{\xi} & \tilde{\eta} \\ -\tilde{\eta} & \tilde{\xi} \end{bmatrix}, \quad \tilde{d} = c\xi\tilde{\eta} + (d\xi - \eta/c)\tilde{\xi},$$

and

$$\tilde{t}_3 = \xi t_3 + \frac{\eta}{c} e^{-i\theta} t_4, \qquad t_4 = T_1^{-1} t_1.$$

Since T_1 is upper triangular, t_4 can be computed with a back substitution.

In the second case, partition the old blocks T_{11} and W as

$$T_{11} := \begin{bmatrix} T_1 & t_1 \\ 0 & ce^{i\theta} \end{bmatrix}, \quad W := \begin{bmatrix} W_1 & w_2 \\ w_2^* & w_{nn} \end{bmatrix}, \quad W_1 = W_1^*.$$

Direct calculations yield the following update formulas for the new T_{11} and W:

$$\begin{bmatrix} T_1 & \tilde{\xi} t_1 - \tilde{\eta}\tilde{w}_2 \\ 0 & r^{-1}e^{i\theta} \end{bmatrix} \to T_{11},$$

$$\begin{bmatrix} W_1 - \tilde{w}_2 t_1^* + (\tilde{\eta} t_1 + \tilde{\xi}\tilde{w}_2)(\tilde{\xi} t_1 - \tilde{\eta}\tilde{w}_2)^* & r^{-1}e^{-i\theta}(\tilde{\eta} t_1 + \tilde{\xi}\tilde{w}_2) \\ r^{-1}e^{i\theta}(\tilde{\eta} t_1 + \tilde{\xi}\tilde{w}_2)^* & r^{-1}(c\xi\tilde{\eta} + c^{-1}(w_{nn}\xi - \eta)\tilde{\xi}) \end{bmatrix} \to W,$$

where $\tilde{w}_2 = c^{-1}e^{i\theta} w_2$, and r, $\tilde{\xi}$, $\tilde{\eta}$ are defined in (3.8) with $d = w_{nn}/c$.

Now, after having computed Δ and $\tilde{\Delta}$,

$$\tilde{\Delta}^T \mathcal{G}_{n-1} \Gamma_n \mathcal{Y}_{n-1} \Delta = \left[\begin{array}{cc|cc} I & & 0 & \\ & M_1 & & M_2 \\ \hline 0 & & I & \\ & -M_2 & & M_1 \end{array}\right],$$

where M_1 and M_2 are 2×2 matrices, and M_2 is rank one. Let $Z_{n-1}, G_{n-1} \in \mathbb{G}_{n-1}$ be Givens rotations so that the $(n, n-1)$ entries in both of the matrices

$$\begin{bmatrix} 0 & \\ & M_2 \end{bmatrix} Z_{n-1}, \quad G_{n-1}^* \begin{bmatrix} I & \\ & M_1 \end{bmatrix} Z_{n-1}$$

are zero, the (n,n) entry of the first matrix is real, and the $(n-1,n-1)$ entry of the second matrix is positive. From the unitary symplectic property and the fact that M_2 is rank one, for

$$\mathcal{Z}_{n-1} = \begin{bmatrix} Z_{n-1} & 0 \\ 0 & Z_{n-1} \end{bmatrix} \quad \text{and} \quad \mathcal{G}_{n-1} = \begin{bmatrix} G_{n-1} & 0 \\ 0 & G_{n-1} \end{bmatrix},$$

$$\mathcal{G}_{n-1}^* \left[\begin{array}{cc|cc} I & & 0 & \\ & M_1 & & M_2 \\ \hline 0 & & I & \\ & -M_2 & & M_1 \end{array}\right] \mathcal{Z}_{n-1} =: \left[\begin{array}{cc|cc} I & & 0 & \\ & \phi & & \psi \\ \hline 0 & & I & \\ & -\psi & & \phi \end{array}\right] = \Gamma_n(\phi,\psi) =: \Gamma_n,$$

where ϕ, ψ are real and $\phi^2+\psi^2=1$. So we have the forms

$$\tilde{\Delta}^T \mathcal{G}_{n-1}\Gamma_n \mathcal{Y}_{n-1}\Delta =: \mathcal{G}_{n-1}\Gamma_n \mathcal{Z}_{n-1}^*$$

and

$$\Delta^T \mathcal{Y}^* \mathcal{S} \mathcal{Y} \Delta =: \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n \mathcal{Z}_{n-1}^*.$$

We are now ready to perform the transformation with $\mathcal{Z}$ by taking $\mathcal{Z}_{n-1}$ as the starting symplectic Givens rotation. Clearly,

$$\mathcal{Z}_{n-1}^* \Delta^T \mathcal{Y}^* \mathcal{S}\mathcal{Y}\Delta \mathcal{Z}_{n-1} = \mathcal{Z}_{n-1}^* \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n =: \mathcal{Z}_{n-1}^* \mathcal{T}\mathcal{G}\Gamma_n. \tag{3.9}$$

Similarly, the matrix $Z = Z_{n-1}\dots Z_1$ can be determined by running the core-chasing process on $T_{11}G$ but in the reversed order. The goal is to transform $Z_{n-1}^* T_{11} G$ back to a factored form as $T_{11}G$. First of all, we determine a Givens rotation $\tilde{Z}_{n-1} \in \mathbb{G}_{n-1}$ such that $T_{11} := Z_{n-1}^* T_{11} \tilde{Z}_{n-1}^*$ is upper triangular. Then

$$Z_{n-1}^* T_{11} G =: T_{11}\tilde{Z}_{n-1} G_1 \dots, G_{n-1} = T_{11} G_1 \dots G_{n-3} \tilde{Z}_{n-1} G_{n-2} G_{n-1}.$$

The product $\tilde{Z}_{n-1}G_{n-2}G_{n-1}$ can be expressed as $G_{n-2}G_{n-1}Z_{n-2}^*$ with a turnover, where $G_{n-2}, Z_{n-2} \in \mathbb{G}_{n-2}$ and $G_{n-1} \in \mathbb{G}_{n-1}$. Then

$$Z_{n-1}^* T_{11} G = T_{11} G_1 \dots G_{n-3} G_{n-2} G_{n-1} Z_{n-2}^*$$

and

$$\begin{aligned} Z_{n-2}^* Z_{n-1}^* T_{11} G Z_{n-2} &= Z_{n-2}^* T_{11} G_1 \dots G_{n-3} G_{n-2} G_{n-1} \\ &=: T_{11} G_1 \dots G_{n-4} \tilde{Z}_{n-2} G_{n-3} G_{n-2} G_{n-1} \end{aligned}$$

for some $\tilde{Z}_{n-2} \in \mathbb{G}_{n-2}$ such that $T_{11} := Z_{n-2}^* T_{11} \tilde{Z}_{n-2}^*$ is upper triangular. Similarly, the product $\tilde{Z}_{n-2}G_{n-3}G_{n-2}$ can be expressed as $G_{n-3}G_{n-2}Z_{n-3}^*$ for some $G_{n-3}, Z_{n-3} \in \mathbb{G}_{n-3}$, and $G_{n-2} \in \mathbb{G}_{n-2}$. So

$$\begin{aligned} Z_{n-2}^* Z_{n-1}^* T_{11} G Z_{n-2} &=: T_{11} G_1 \dots G_{n-3} G_{n-2} Z_{n-3}^* G_{n-1} \\ &= T_{11} G_1 \dots G_{n-3} G_{n-2} G_{n-1} Z_{n-3}^*. \end{aligned}$$

Continue this core-chasing process until one has

$$Z_1^* \dots Z_{n-1}^* T_{11} G Z_{n-2} \dots Z_1 = Z_1^* T_{11} G_1 \dots G_n.$$

One can determine $\tilde{Z}_1 \in \mathbb{G}_1$ such that $T_{11} := Z_1^* T_{11} \tilde{Z}_1^*$ is upper triangular. Setting $G_1 := \tilde{Z}_1 G_1 \in \mathbb{G}_1$, one has

$$Z_1^* \dots Z_{n-2}^* Z_{n-1}^* T_{11} G Z_{n-2} \dots Z_1 = T_{11} G_1 \dots G_n =: T_{11} G.$$

Let

$$\mathcal{Z}_i = \begin{bmatrix} Z_i & 0 \\ 0 & Z_i \end{bmatrix}, \quad \mathcal{G}_i = \begin{bmatrix} G_i & 0 \\ 0 & G_i \end{bmatrix} \in \mathbb{SG}_i, \quad i = n-1, \dots, 1,$$

and define

$$\mathcal{Z} = \mathcal{Z}_{n-1} \dots \mathcal{Z}_1, \quad \mathcal{G} = \mathcal{G}_1 \dots \mathcal{G}_{n-1}.$$

Let

$$\mathcal{T} = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix}$$

with T_{11} being updated as above and T_{12}, T_{22} being updated with the same transformations. Following (3.9), the above constructions, and the fact that Γ_n commutes with $\mathcal{Z}_i$ for $i = n-2, \dots, 1$, one has that for $\mathcal{Q} = \mathcal{Y}\Delta\mathcal{Z}$,

$$\mathcal{Q}^* \mathcal{S} \mathcal{Q} = \mathcal{Z}^* \Delta^T \mathcal{Y}^* \mathcal{S} \mathcal{Y} \Delta \mathcal{Z} = \mathcal{T} \mathcal{G} \Gamma_n,$$

which is again in the factored form (3.1). This completes one single shift symplectic QR iteration. Note each $\tilde{Z}_i$ also restores the lower triangular form of $Z_i^* T_{22}$ in the iteration. So in order to preserve the error order, $\tilde{Z}_i$ should be determined either by the $(i+1, i)$, $(i+1, i+1)$ entires of $Z_i^* T_{11}$ or the (i, i), $(i, i+1)$ entries of $Z_i^* T_{22}$, as did for Y_i in the first part. Also, economic versions of the iteration can be constructed in the same way as the first part but with the reversed order.

If the old $\mathcal{T}$ is a symplectic upper triangular matrix plus an error of order $O(\|\mathcal{T}\|\mathbf{u})$, using the above mentioned strategy for determining $\mathcal{Y}_i$, $\tilde{\mathcal{Z}}_i$, and $\Delta, \tilde{\Delta}$ (assuming that the replacement will not introduce large errors), one can show that the updated $\mathcal{T}$ after one core-chasing symplectic single shift QR iteration is still a symplectic upper triangular matrix plus an error of order $O(\|\mathcal{T}\|\mathbf{u})$. So the iteration is backward stable. In general, the two economic iterations are unable to achieve the same kind of backward stability. In both cases, one still needs to use $T_{22} = T_{11}^{-*}$ and in the second case, the iteration is always carried out on $W = T_{12} T_{11}^*$.

The main work of one core-chasing symplectic single shift QR iteration is for updating the symplectic upper triangular matrix $\mathcal{T}$. For the transformations with $\mathcal{Y}$ and $\mathcal{Z}$ one only needs to compute $Y_i^* T_{k\ell} \tilde{Y}_i^*$, $Z_i^* T_{k\ell} \tilde{Z}_i$ for $1 \le k \le \ell \le 2$ and $i = 1, 2, \dots, n-1$, which requires $48n^2$ flops. The two economic versions require $37n^2$ and $26n^2$ flops, respectively. The iteration provided in [20] costs about $60n^2$ flops. If the unitary symplectic similarity matrix needs to be computed, it needs additional $24n^2$ flops per iteration for all four iteration methods. Recall that a unitary symplectic matrix has a block form

$$\begin{bmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{bmatrix}.$$

So it suffices to compute U_1 and U_2.

3.3. Choices of shifts and stopping criterion. The shift σ can be chosen as s_{11}, the $(1,1)$ entry of $\mathcal{S}$ (a Rayleigh quotient shift), or the eigenvalue of the 2×2 leading principal submatrix of $\mathcal{S}$ that is closer to s_{11} (a Wilkinson's shift). Note when $\mathcal{S}$ is in the factored form (3.1), the 2×2 leading principal submatrix is

$$[e_1, e_2]^T \mathcal{T} \mathcal{G}_1 \mathcal{G}_2 [e_1, e_2] = \begin{bmatrix} t_{11}\alpha_1 - t_{12}\bar{\beta}_1 & (t_{11}\beta_1 - t_{12}\bar{\alpha}_1)\alpha_2 \\ -t_{22}\bar{\beta}_1 & t_{22}\bar{\alpha}_1\alpha_2 \end{bmatrix}$$

with $\mathcal{G}_i = \mathcal{G}_i(\alpha_i, \beta_i)$ and $t_{ij} = e_i^* \mathcal{T} e_j$ for $1 \le i \le j \le 2$. So σ is either $t_{11}\alpha_1 - t_{12}\bar{\beta}_1$ or one of the eigenvalues of the above 2×2 matrix that is closer to $t_{11}\alpha_1 - t_{12}\bar{\beta}_1$.

During the iterations, it is expected that β_1 from G_1 or $\mathcal{G}_1$ will converge to zero first. When it is sufficiently small we set $\mathcal{G}_1$ to be diagonal and update $\mathcal{T} := \mathcal{T}\mathcal{G}_1$. We then continue the iteration on the part related to $\mathcal{G}_2, \ldots, \mathcal{G}_{n-1}$, and so on. If during the iterations η in Γ_n converges to zero, we set Γ_n to be diagonal and $\mathcal{T}\mathcal{G}\Gamma_n$ is block upper triangular. We then simply implement the standard core-chasing iterations on the remaining upper Hessenberg part of the $(1,1)$ block, which is part of $T_{11}G$, for the rest of the iterations. If all $\mathcal{G}_1, \ldots, \mathcal{G}_{n-1}$ eventually become diagonal, $\mathcal{S}$ will be transformed to a matrix of the form $\mathcal{T}\Gamma_n$. If the eigenvalues of

$$\begin{bmatrix} t_{nn} & t_{n,2n} \\ 0 & \bar{t}_{nn}^{-1} \end{bmatrix} \begin{bmatrix} \phi & \psi \\ -\psi & \phi \end{bmatrix}$$

are not unimodular, then $\mathcal{T}\Gamma_n$ can be transformed to a symplectic upper triangular form using a similarity transformation with a symplectic Givens rotation from $\mathbb{SG}_n$. In this case, $\mathcal{S}$ has a symplectic Schur form. If the eigenvalues of the above 2×2 matrix are unimodular, the above transformation might still exist. If not, $\mathcal{S}$ does not have a symplectic Schur form [19] and we stop the algorithm without performing further transformations. The deflation criterion for a core-chasing iteration is simple. That is one of the main advantages of using a core-chasing iteration. We may simply set $|\beta_i|, |\eta| < C(n)\mathbf{u}$, where $C(n)$ is a certain lower degree polynomial of n. With such a criterion, errors introduced by the deflation are of order $C(n)\|\mathcal{S}\|\mathbf{u}$. Note the iteration may stagnate if σ is unimodular. This is because $(\mathcal{S} - \sigma I)^{-1}(\bar{\sigma}\mathcal{S} - I) = \bar{\sigma} I$ if $|\sigma| = 1$ and the Q factor of its symplectic QR factorization is I. Stagnation must happen when $\mathcal{S}$ has more than two unimodular eigenvalues. In this case, we may switch to a different shift or use a constant shift (say 0) until a deflation happens. If the stagnation still occurs, it indicates that $\mathcal{S}$ may not have a symplectic Schur form. So we stop the iteration.

3.4. Numerical examples. We tested the proposed single shift symplectic QR algorithm and its two economic versions on 100 randomly generated 60×60 symplectic matrices satisfying the condition (2.3). All of the numerical computations were carried out with MATLAB R2017a on an iMac with a 2.8 GHz Intel Core i5 processor. Each matrix is generated by the formula

$$\mathcal{S} = \begin{bmatrix} X_1 & 0 \\ 0 & X_1^{-*} \end{bmatrix} \begin{bmatrix} I & (X_3 + X_3^*)/2 \\ 0 & I \end{bmatrix} \Gamma_{30}(a, b) \begin{bmatrix} X_2 & 0 \\ 0 & X_2^{-*} \end{bmatrix},$$

where X_1 X_2, X_3 are 30×30 generated by MATLAB command `randn(30)+i*randn(30)`; $b = \sqrt{1 - a^2}$, and a is generated by the MATLAB command `rand(1)`. The norms of these 100 matrices are of order 10^3. All of the computational results that are from the three versions of the proposed algorithm will be labeled with W(hole), H(alf), F(actored), respectively, representing the full matrix version algorithm, the first and second economic versions. The results from Mehrmann's algorithm in [20] will be labeled with M. For all four algorithms we used the Wilkinson's shift. For the first three algorithms we used the stopping criterion as described in the previous subsection with $C(n) = n$. For Algorithm M we used the stopping criterion $|s_{j+1,j}| < (|s_{jj}| + |s_{j+1,j+1}|)n\mathbf{u}$, where s_{ij} is the (i,j) entry of the $(1,1)$ block of a symplectic upper Hessenberg form.

On average, Algorithms W, P, F consume more CPU time than Algorithm M. The averages of the CPU time are 0.341, 0.282, 0.317, and 0.125 seconds, respectively. The

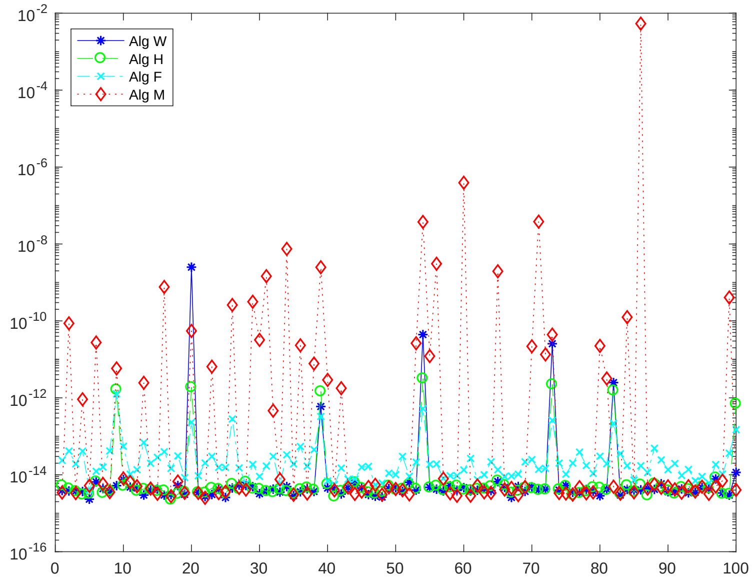

Fig. 1. *Residuals of the Schur forms computed by four algorithms.*

main reason is that Algorithm M uses matrix-matrix and matrix-vector operations more efficiently than the proposed algorithms.

For each algorithm and each symplectic matrix, let the computed symplectic Schur form be $\mathcal{Q}\mathcal{T}\mathcal{Q}^*$, where $\mathcal{Q}$ and $\mathcal{T}$ are the computed unitary symplectic matrix and symplectic upper triangular matrix, respectively. We computed the residual $\|\mathcal{S} - \mathcal{Q}\mathcal{T}\mathcal{Q}^*\|/\|\mathcal{S}\|$. Note that $\mathcal{T}$ resulting from the first three algorithms will still be in a factored form (3.1) if the algorithms fail to compute a symplectic Schur form. All of the residuals are plotted in Figure 1. In many cases the residuals from all four algorithms are of order $O(10^{-15})$. Algorithm M produces much bigger residuals for one-third of the matrices. Algorithms W and H behave quite similarly and provide small residuals most of the time. The residuals from Algorithm F are usually larger than the rest, but they change quite mildly. We report that among all 100 matrices five cause a stagnation for all four algorithms.

3.5. QR iteration: Double shift case. The core-chasing procedure for the double shift symplectic QR iteration can also be developed following the one given in [20]. One main reason for introducing the double shift QR iteration is the use of real arithmetic when $\mathcal{S}$ is real, although it works for complex matrices as well. When a symplectic matrix is real, it is easily seen that a real version of the factored form (3.1) can be obtained in exactly the same way. So in this subsection we assume that $\mathcal{S}$ is real and already in the factored form (3.1).

We write

$$\Gamma_n = \begin{bmatrix} D_1 & D_2 \\ -D_2 & D_1 \end{bmatrix}, \quad D_1 = \begin{bmatrix} I & 0 \\ 0 & \phi \end{bmatrix}, \quad D_2 = \begin{bmatrix} 0 & 0 \\ 0 & \psi \end{bmatrix}, \quad \mathcal{G} = \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix},$$

where

$$G = G_1 \dots G_{n-1}, \quad G_i \in \mathbb{G}_i, \quad i = 1, \dots, n-1,$$

and define

$$F := T_{11}G, \quad K := T_{12}G.$$

Note that F is upper Hessenberg. Then $T_{22}G = T_{11}^{-T}G = F^{-T}$ and

$$\mathcal{S} = \begin{bmatrix} FD_1 - KD_2 & FD_2 + KD_1 \\ -F^{-T}D_2 & F^{-T}D_1 \end{bmatrix} =: \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}.$$

The double shift symplectic QR iteration for $\mathcal{S}$ is based on a symplectic QR factorization of the real symplectic matrix

$$(\mathcal{S} - \sigma_1 I)^{-1}(\mathcal{S} - \sigma_2 I)^{-1}(\sigma_1 \mathcal{S} - I)(\sigma_2 \mathcal{S} - I) = (\mathcal{S}^2 - \mu\mathcal{S} + \nu I)^{-1}(\nu\mathcal{S}^2 - \mu\mathcal{S} + I), \tag{3.10}$$

where the shifts σ_1, σ_2 are either both real or $\sigma_2 = \bar{\sigma}_1$, and $\mu = \sigma_1 + \sigma_2$, $\nu = \sigma_1\sigma_2$. As in [20], we need to show the block structures of the matrices $\mathcal{S}^2 - \mu\mathcal{S} + \nu I$ and $\nu\mathcal{S}^2 - \mu\mathcal{S} + I$, since they are critical for the construction of the QR iteration. Define

$$\mathcal{K} := \begin{bmatrix} I & 0 \\ 0 & (F^T)^2 \end{bmatrix} (\mathcal{S}^2 - \mu\mathcal{S} + \nu I) = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix},$$
$$\mathcal{L} := \begin{bmatrix} I & 0 \\ 0 & (F^T)^2 \end{bmatrix} (\nu\mathcal{S}^2 - \mu\mathcal{S} + I) = \begin{bmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{bmatrix}.$$

Then $(\mathcal{S}^2 - \mu\mathcal{S} + \nu I)^{-1}(\nu\mathcal{S}^2 - \mu\mathcal{S} + I) = \mathcal{K}^{-1}\mathcal{L}$, and using the block form of $\mathcal{S}$, one has

$$\begin{aligned}
K_{11} &= S_{11}^2 - \mu S_{11} + \nu I + S_{12}S_{21}, \\
K_{12} &= S_{11}S_{12} + S_{12}S_{22} - \mu S_{12}, \\
K_{21} &= (F^T)^2(S_{21}S_{11} + S_{22}S_{21} - \mu S_{21}) \\
&= F^T(D_2KD_2 + \tilde{D}_1F^{-T}D_2 + \mu D_2 - D_2FD_1) - D_2, \\
K_{22} &= (F^T)^2(S_{22}^2 - \mu S_{22} + \nu I + S_{21}S_{12}) \\
&= (\nu F^2 - \mu F + I)^T + e_{n-1}k_1^T + e_n k_2^T, \\
L_{11} &= \nu S_{11}^2 - \mu S_{11} + I + \nu S_{12}S_{21} = \nu F^2 - \mu F + I + \ell_1 e_{n-1}^T + \ell_2 e_n^T, \\
L_{12} &= \nu(S_{11}S_{12} + S_{12}S_{22}) - \mu S_{12}, \\
L_{21} &= (F^T)^2(\nu(S_{21}S_{11} + S_{22}S_{21}) - \mu S_{21}) \\
&= F^T(\nu D_2KD_2 + \nu\tilde{D}_1F^{-T}D_2 + \mu D_2 - \nu D_2FD_1) - \nu D_2, \\
L_{22} &= (F^T)^2(\nu S_{22}^2 - \mu S_{22} + I + \nu S_{21}S_{12}) \\
&= (F^2 - \mu F + \nu I)^T + e_{n-1}\ell_3^T + e_n\ell_4^T,
\end{aligned} \tag{3.11}$$

where $k_1, k_2, \ell_1, \ell_2, \ell_3, \ell_4 \in \mathbb{R}^n$ and

$$\tilde{D}_1 = I - D_1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 - \phi \end{bmatrix}.$$

Let $\hat{Y}$ be the Q factor of a QR factorization of L_{11}. Because $S_{12}S_{21}$ is zero except the last column, $\hat{Y}$ is also the Q factor of a QR factorization of $\nu S_{11}^2 - \mu S_{11} + I$. Since S_{11} is upper Hessenberg, by viewing $\hat{Y}$ as generated from running one double shift

QR iteration on S_{11}, we have that $\hat{Y}$ is upper t-Hessengberg and $\hat{Y}^T S_{11}\hat{Y}$ is upper Hessenberg. This implies

$$\hat{Y}^T K_{11}\hat{Y} = (\hat{Y}^T S_{11}\hat{Y})^2 - \mu\hat{Y}^T S_{11}\hat{Y} + \nu I + \hat{Y}^T S_{12}S_{21}\hat{Y}$$

is upper t-Hessenberg. From the expressions of L_{11}, the leading $n-2$ columns of $\nu S_{11}^2 - \mu S_{11} + I$ and $\nu F^2 - \mu F + I$ are identical. If Y is the Q factor of a QR factorization of the latter, which is also upper t-Hessenberg, then $Y^T L_{11}$ is upper triangular plus a nonzero $(n, n-1)$ entry. So one may express $\hat{Y} = Y\hat{Y}_{n-1}$ for some $\hat{Y}_{n-1} \in \mathbb{G}_{n-1}$. Hence

$$\hat{Y}^T K_{22}^T = \hat{Y}_{n-1}^T Y^T(\nu F^2 - \mu F + I) + \hat{Y}^T(k_1 e_{n-1}^T + k_2 e_n^T)$$

is upper triangular plus a nonzero $(n, n-1)$ entry. Because F is upper Hessenberg, L_{22} is lower t-Hessenberg, and the blocks K_{21}, L_{21} are zero but a nonzero 2×2 trailing principal submatrix. If we use Y instead of $\hat{Y}$, defining

$$\mathcal{Y} = \begin{bmatrix} Y & 0 \\ 0 & Y \end{bmatrix} \quad \text{and} \quad \hat{\mathcal{Y}} = \begin{bmatrix} Y & 0 \\ 0 & I \end{bmatrix},$$

and from the relation $\hat{Y} = Y\hat{Y}_{n-1}$, we have the following condensed forms:

$$\tilde{\mathcal{K}} = \hat{\mathcal{Y}}^T\mathcal{K}\mathcal{Y} = \left[\begin{array}{cccccc|cccccc}
* & \cdots & * & * & * & * & * & \cdots & \cdots & \cdots & * & * \\
* & \cdots & * & * & * & * & \vdots & & & & \vdots & \vdots \\
* & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & & & & \vdots & \vdots \\
 & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & & & & \vdots & \vdots \\
 & & * & * & * & * & * & \cdots & \cdots & \cdots & * & * \\
 & & + & * & * & * & * & \cdots & \cdots & \cdots & * & * \\
\hline
 & & & & & & * & & & & & \\
 & & & & & & \vdots & \ddots & & & & \\
 & & & & & & \vdots & & \ddots & & & \\
 & & & & & & \vdots & & & \ddots & & \\
 & & * & * & * & * & * & \cdots & \cdots & \cdots & * & * \\
 & & * & * & * & * & * & \cdots & \cdots & \cdots & * & *
\end{array}\right] \tag{3.12}$$

$$\tilde{\mathcal{L}} = \hat{\mathcal{Y}}^T\mathcal{L} = \left[\begin{array}{cccccc|cccccc}
* & \cdots & * & * & * & * & * & \cdots & \cdots & \cdots & * & * \\
 & \ddots & & & & \vdots & \vdots & & & & & \vdots \\
 & & \ddots & & & \vdots & \vdots & & & & & \vdots \\
 & & & \ddots & & \vdots & \vdots & & & & & \vdots \\
 & & & & * & * & * & \cdots & \cdots & \cdots & * & * \\
 & & & & + & * & * & \cdots & \cdots & \cdots & * & * \\
\hline
 & & & & & & * & * & * & & & \\
 & & & & & & \vdots & \ddots & \ddots & \ddots & & \\
 & & & & & & \vdots & & \ddots & \ddots & * & \\
 & & & & & & * & \cdots & \cdots & \ddots & * & * \\
 & & & & * & * & * & \cdots & \cdots & \cdots & * & * \\
 & & & & * & * & * & \cdots & \cdots & \cdots & * & *
\end{array}\right], \tag{3.13}$$

where the two entries marked with "+" are zero if Y is replaced by $\hat{Y}$.

The real orthogonal matrix Y can be determined by performing a standard implicit double shift QR iteration on F with the shifts σ_1^{-1} and σ_2^{-1}. Note that the above condensed form will not change if Y is replaced by YG_{n-1} with an arbitrary $G_{n-1} \in \mathbb{G}_{n-1}$. So we may take Y as the one obtained from the above QR iteration by skipping the last step with a Givens rotation from $\mathbb{G}_{n-1}$ for annihilating the $(n, n-2)$ entry in the bulge chasing process.

In order to obtain a symplectic QR factorization for the matrix (3.10), the next step is to transform $\tilde{\mathcal{L}}$ to a block upper triangular matrix by premultiplying five $2n\times 2n$ (not necessarily symplectic) Givens rotations $\mathcal{N}_1, \mathcal{N}_4 \in \mathbb{G}_{2n-1}$, $\mathcal{N}_2 \in \mathbb{G}_{n-1,2n-1}$, $\mathcal{N}_3 \in \mathbb{G}_{n-1}$, and $\mathcal{N}_5 \in \mathbb{G}_{n,2n-1}$ to annihilate the $(2n, n-1)$, $(2n-1, n-1)$, $(n, n-1)$, $(2n, n)$, $(2n-1, n)$ entries of $\tilde{\mathcal{L}}$, respectively. Then

$$\tilde{\mathcal{L}} := \mathcal{N}_5\mathcal{N}_4\mathcal{N}_3\mathcal{N}_2\mathcal{N}_1\tilde{\mathcal{L}} = \begin{bmatrix} \tilde{L}_{11} & \tilde{L}_{12} \\ 0 & \tilde{L}_{22} \end{bmatrix},$$

where $\tilde{L}_{11}$ is upper triangular and $\tilde{L}_{22}$ is lower t-Hessenberg. The matrix $\tilde{\mathcal{K}} := \mathcal{N}_5\mathcal{N}_4\mathcal{N}_3\mathcal{N}_2\mathcal{N}_1\tilde{\mathcal{K}}$ has the same zero pattern as the old $\tilde{\mathcal{K}}$. For the new pair $(\tilde{\mathcal{L}}, \tilde{\mathcal{K}})$, the matrix $\tilde{\mathcal{K}}^{-1}\tilde{\mathcal{L}}$ is still a symplectic matrix. So is its inverse $\tilde{\mathcal{L}}^{-1}\tilde{\mathcal{K}}$. Using the fact that the $(2, 2)$ block of $(\tilde{\mathcal{L}}^{-1}\tilde{\mathcal{K}})\mathcal{J}_n(\tilde{\mathcal{L}}^{-1}\tilde{\mathcal{K}})^T$ must be zero, the $(2, 1)$ block of the new $\tilde{\mathcal{K}}$ is zero but a nonzero 2×2 trailing principal submatrix. We then determine four symplectic Givens rotations $\mathcal{X}_1, \mathcal{X}_2 = \mathbb{SG}_{n-1}$, and $\Delta_1, \Delta_2 = \mathbb{SG}_n$, and postmultiply them to the new $\tilde{\mathcal{K}}$ to annihilate the $(2n-1, n-1)$, $(2n-1, n)$, $(2n, n-1)$ (or $(2n-1, 2n)$), and $(2n, n)$ entries. For $\Theta = \mathcal{X}_1\Delta_1\mathcal{X}_2\Delta_2$, the symplectic property ensures

$$\tilde{\mathcal{K}}\Theta = \begin{bmatrix} \tilde{K}_{11} & \tilde{K}_{12} \\ 0 & \tilde{K}_{22} \end{bmatrix},$$

where the block $\tilde{K}_{11}$ is upper t-Hessenberg (the $(n, n-3)$ entry becomes zero) and $\tilde{K}_{22}$ is lower triangular. Finally, let Z be a real orthogonal matrix such that $\tilde{K}_{11}Z$ is upper triangular. Then for

$$\mathcal{Z} = \begin{bmatrix} Z & 0 \\ 0 & Z \end{bmatrix},$$

the matrix

$$\begin{aligned}(\mathcal{Y}\Theta\mathcal{Z})^T(\mathcal{S}^2 - \mu\mathcal{S} + \nu I)^{-1}(\nu\mathcal{S}^2 - \mu\mathcal{S} + I) &= (\mathcal{Y}\Theta\mathcal{Z})^T\mathcal{K}^{-1}\mathcal{L} \\ &= (\mathcal{N}_4\mathcal{N}_3\mathcal{N}_2\mathcal{N}_1\hat{\mathcal{Y}}^T\mathcal{K}\mathcal{Y}\Theta\mathcal{Z})^{-1}(\mathcal{N}_4\mathcal{N}_3\mathcal{N}_2\mathcal{N}_1\hat{\mathcal{Y}}^T\mathcal{L})\end{aligned}$$

must be symplectic upper triangular. Therefore, a double shift symplectic QR iteration concerns performing the similarity transformation

$$(\mathcal{Y}\Theta\mathcal{Z})^T\mathcal{S}(\mathcal{Y}\Theta\mathcal{Z}),$$

which can be done following the order $\mathcal{S} := \mathcal{Y}^T\mathcal{S}\mathcal{Y}$, $\mathcal{S} := \Theta^T\mathcal{S}\Theta$, and $\mathcal{S} := \mathcal{Z}^T\mathcal{S}\mathcal{Z}$.

As described above, the transformation $\mathcal{Y}^T\mathcal{S}\mathcal{Y}$ is essentially determined by performing a double shift QR iteration on the matrix $F = T_{11}G$ with the shifts σ_1^{-1} and σ_2^{-1} that generates an orthogonal matrix Y so that Y^TFY is upper Hessenberg plus a nonzero $(n, n-2)$ entry. The matrix Y can be expressed as a product of Givens rotations and can be generated with a core-chasing iteration process. The first two Givens rotations are $Y_1 \in \mathbb{G}_1, P_2 \in \mathbb{G}_2$ satisfying

$$Y_1^TP_2^T(\nu F^2 - \mu F + I)e_1 = Y_1^TP_2^T(\nu T_{11}G_1G_2T_{11}G_1e_1 - \mu T_{11}G_1e_1 + e_1) \in \operatorname{span}\{e_1\}.$$

We perform the orthogonal similarity transformation

$$Y_1^T P_2^T F P_2 Y_1 = Y_1^T P_2^T T_{11} G P_2 Y_1 = Y_1^T P_2^T T_{11} G_1 G_2 G_3 P_2 Y_1 G_4 \dots G_{n-1}.$$

First, there exist $\tilde{P}_2 \in \mathbb{G}_2$ and $\tilde{Y}_1 \in \mathbb{G}_1$ so that $T_{11} := Y_1^T P_2^T T_{11} \tilde{P}_2^T \tilde{Y}_1^T$ is still upper triangular. So

$$Y_1^T P_2^T F P_2 Y_1 =: T_{11} \tilde{Y}_1 \tilde{P}_2 G_1 G_2 G_3 P_2 Y_1 G_4 \dots G_{n-1}.$$

Performing the turnovers on the product $\tilde{Y}_1 \tilde{P}_2 G_1 G_2 G_3 P_2 Y_1$ with

$$\begin{aligned}(\mathbf{1}, \mathbf{2}, \mathbf{1}, 2, 3, 2, 1) &\to (2, 1, \mathbf{2}, \mathbf{2}, 3, 2, 1) \to (2, 1, \mathbf{2}, \mathbf{3}, \mathbf{2}, 1) \to (2, \mathbf{1}, \mathbf{3}, 2, \mathbf{3}, \mathbf{1})\\ &= (2, 3, \mathbf{1}, \mathbf{2}, \mathbf{1}, 3) \to (\mathbf{2}, \mathbf{3}, \mathbf{2}, 1, 2, 3) \to (3, 2, \mathbf{3}, \mathbf{1}, 2, 3) = (3, 2, 1, 3, 2, 3),\end{aligned}$$

i.e.,

$$\tilde{Y}_1 \tilde{P}_2 G_1 G_2 G_3 P_2 Y_1 =: \tilde{P}_3 \tilde{Y}_2 G_1 \tilde{G}_3 G_2 G_3 \quad G_1 \in \mathbb{G}_1, \quad \tilde{Y}_2, G_2 \in \mathbb{G}_2, \quad \tilde{P}_3, \tilde{G}_3, G_3 \in \mathbb{G}_3.$$

Then

$$Y_1^T P_2^T F P_2 Y_1 =: T_{11} \tilde{P}_3 \tilde{Y}_2 G_1 \tilde{G}_3 G_2 G_3 G_4 \dots G_{n-1}.$$

Next, one can determine two Givens rotations $P_3 \in \mathbb{G}_3, Y_2 \in \mathbb{G}_2$ such that $T_{11} := Y_2^T P_3^T T_{11} \tilde{P}_3 \tilde{Y}_2$ is upper triangular, and then perform the similarity transformation

$$Y_2^T P_3^T Y_1^T P_2^T F P_2 Y_1 P_3 Y_2 =: T_{11} G_1 \tilde{G}_3 G_2 G_3 G_4 P_3 Y_2 G_5 \dots G_{n-1}.$$

For the product $G_1 \tilde{G}_3 G_2 G_3 G_4 P_3 Y_2$, we take the following turnovers:

$$\begin{aligned}(1, 3, 2, \mathbf{3}, \mathbf{4}, \mathbf{3}, 2) &\to (1, 3, \mathbf{2}, \mathbf{4}, 3, \mathbf{4}, \mathbf{2}) = (1, 3, 4, \mathbf{2}, \mathbf{3}, \mathbf{2}, 4) \to (1, \mathbf{3}, \mathbf{4}, \mathbf{3}, 2, 3, 4)\\ &\to (\mathbf{1}, \mathbf{4}, 3, \mathbf{4}, \mathbf{2}, 3, 4) = (4, \mathbf{1}, \mathbf{3}, 2, 4, 3, 4) \to (4, 3, 1, 2, 4, 3, 4).\end{aligned}$$

So

$$Y_2^T P_3^T Y_1^T P_2^T F P_2 Y_1 P_3 Y_2 =: T_{11} \tilde{P}_4 \tilde{Y}_3 G_1 G_2 \tilde{G}_4 G_3 G_4 G_5 \dots G_{n-1}.$$

Similarly, there are $P_4 \in \mathbb{G}_4, Y_3 \in \mathbb{G}_3$ such that $T_{11} := Y_3^T P_4^T T_{11} \tilde{P}_4 \tilde{Y}_3$ is upper triangular and

$$Y_2^T P_3^T Y_1^T P_2^T F P_2 Y_1 P_3 Y_2 =: P_4 Y_3 T_{11} G_1 G_2 \tilde{G}_4 G_3 G_4 \dots G_{n-1}.$$

We continue the process until we have

$$Y_{n-3}^T P_{n-2}^T \dots P_2^T F P_2 \dots P_{n-2} Y_{n-3} =: P_{n-1} Y_{n-2} T_{11} G_1 \dots G_{n-3} \tilde{G}_{n-1} G_{n-2} G_{n-1}.$$

Then for

$$Y = P_2 Y_1 \dots P_{n-2} Y_{n-3} P_{n-1} Y_{n-2},$$

the matrix

$$\tilde{F} := Y^T F Y =: T_{11} G_1 \dots G_{n-3} \tilde{G}_{n-1} G_{n-2} G_{n-1} P_{n-1} Y_{n-2} \tag{3.14}$$

is upper Hessenberg plus a nonzero $(n, n-2)$ entry. Defining

$$\mathcal{Y}_i = \begin{bmatrix} Y_i & 0 \\ 0 & Y_i \end{bmatrix}, \ \mathcal{P}_i = \begin{bmatrix} P_i & 0 \\ 0 & P_i \end{bmatrix}, \ \mathcal{G}_i = \begin{bmatrix} G_i & 0 \\ 0 & G_i \end{bmatrix}, \ \tilde{\mathcal{G}}_{n-1} = \begin{bmatrix} \tilde{G}_{n-1} & 0 \\ 0 & \tilde{G}_{n-1} \end{bmatrix},$$

and

$$\mathcal{Y} = \mathcal{P}_2\mathcal{Y}_1 \ldots \mathcal{P}_{n-2}\mathcal{Y}_{n-3}\mathcal{P}_{n-1}\mathcal{Y}_{n-2} = \begin{bmatrix} Y & 0 \\ 0 & Y \end{bmatrix},$$

one has

$$\begin{aligned} \tilde{\mathcal{S}} &:= \mathcal{Y}^T\mathcal{S}\mathcal{Y} = \mathcal{Y}^T\mathcal{T}\mathcal{G}\Gamma_n\mathcal{Y} \\ &=: \mathcal{T}\mathcal{G}_1 \ldots \mathcal{G}_{n-3}\tilde{\mathcal{G}}_{n-1}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n\mathcal{P}_{n-1}\mathcal{Y}_{n-2} =: \begin{bmatrix} \tilde{S}_{11} & \tilde{S}_{12} \\ \tilde{S}_{21} & \tilde{S}_{22} \end{bmatrix}. \end{aligned} \tag{3.15}$$

Note that $\mathcal{P}_{n-1}$ and Γ_n do not commute. Note also that the blocks T_{12} and T_{22} in the new $\mathcal{T}$ are updated in the same way as for T_{11}, and T_{22} is lower triangular.

Next, we need to determine $\mathcal{X}_1$, Δ_1, $\mathcal{X}_2$, Δ_2 that define Θ. For this we need to determine the Givens rotations $\mathcal{N}_1, \ldots, \mathcal{N}_5$ first. Observe that for constructing all these orthogonal matrices we only need the 2×2 trailing principal submatrices of the four blocks of $\tilde{\mathcal{K}}$ in (3.12) and those of the $(1,1)$ and $(2,1)$ blocks of $\tilde{\mathcal{L}}$ in (3.13). Let $E_n = [e_{n-1}, e_n]$. The $(2,1)$ block of $\tilde{\mathcal{L}}$ is just L_{21} given in (3.11). So its 2×2 trailing principal submatrix is $E_n^T L_{21} E_n$. The 2×2 trailing principal submatrix of the $(1,1)$ block of $\tilde{\mathcal{L}}$ can be computed using the formula

$$E_n^T(\nu\tilde{S}_{11}^2 - \mu\tilde{S}_{11} + I + \nu\tilde{S}_{12}\tilde{S}_{21})Y^T E_n.$$

The 2×2 trailing principal submatrices of the $(1,1)$, $(2,1)$, $(1,2)$, $(2,2)$ blocks of $\tilde{\mathcal{K}}$ can be computed using the formulas

$$E_n^T(\tilde{S}_{11}^2 - \mu\tilde{S}_{11} + \nu I + \tilde{S}_{12}\tilde{S}_{21})E_n, \quad E_n^T K_{21} Y E_n$$

and

$$E_n^T(\tilde{S}_{11}\tilde{S}_{12} + \tilde{S}_{12}\tilde{S}_{22} - \mu\tilde{S}_{12})E_n, \quad E_n^T Y(\tilde{F}^T)^2(\tilde{S}_{22}^2 - \mu\tilde{S}_{22} + \nu I + \tilde{S}_{21}\tilde{S}_{12})E_n,$$

respectively. Here $\tilde{S}_{ij}$, $i,j = 1,2$, are defined in (3.15), $\tilde{F}$ is given in (3.14), and K_{21} is from (3.11). With the above formulas the cost for computing these submatrices is negligible.

Assume that the orthogonal symplectic matrices $\mathcal{X}_1, \mathcal{X}_2$ and Δ_1, Δ_2 are determined. Since $\mathcal{X}_1 \in \mathbb{SG}_{n-1}$, one can determine an orthogonal symplectic matrix $\hat{\mathcal{G}}_{n-1} \in \mathbb{SG}_{n-1}$ such that $\mathcal{T} := \mathcal{X}_1^T\mathcal{T}\hat{\mathcal{G}}_{n-1}^T$ is symplectic upper triangular. By denoting $\tilde{\mathcal{G}}_{n-1} := \hat{\mathcal{G}}_{n-1}\tilde{\mathcal{G}}_{n-1}$, one has

$$\mathcal{X}_1^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\mathcal{X}_1 =: \mathcal{T}\mathcal{G}_1 \ldots \mathcal{G}_{n-3}\tilde{\mathcal{G}}_{n-1}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n\mathcal{P}_{n-1}\mathcal{Y}_{n-2}\mathcal{X}_1.$$

For Δ_1, there is $\tilde{\Delta}_1 \in \mathbb{SG}_n$ such that $\mathcal{T} := \Delta_1^T\mathcal{T}\tilde{\Delta}_1$ stays symplectic upper triangular. Then

$$\Delta_1^T\mathcal{X}_1^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\mathcal{X}_1\Delta_1 =: \mathcal{T}\mathcal{G}_1 \ldots \mathcal{G}_{n-3}\tilde{\Delta}_1^T\tilde{\mathcal{G}}_{n-1}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n\mathcal{P}_{n-1}\mathcal{Y}_{n-2}\mathcal{X}_1\Delta_1.$$

Continue the transformations with $\mathcal{X}_2$ and Δ_2. Eventually, for $\Theta = \mathcal{X}_1\Delta_1\mathcal{X}_2\Delta_2$ we have

$$\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta =: \mathcal{T}\mathcal{G}_1 \ldots \mathcal{G}_{n-3}\mathcal{M},$$

where

$$\mathcal{M} = \tilde{\Delta}_2^T\hat{\mathcal{G}}_{n-1}\tilde{\Delta}_1^T\tilde{\mathcal{G}}_{n-1}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n\mathcal{P}_{n-1}\mathcal{Y}_{n-2}\mathcal{X}_1\Delta_1\mathcal{X}_2\Delta_2 = \left[\begin{array}{cc|cc} I & 0 & 0 & 0 \\ 0 & M_1 & 0 & M_2 \\ \hline 0 & 0 & I & 0 \\ 0 & -M_2 & 0 & M_1 \end{array}\right]$$

is orthogonal and symplectic, and M_1, M_2 are both 3×3. By construction, M_2 must be rank one. So there are Givens rotations $G_{n-2}, Z_{n-2} \in \mathbb{G}_{n-2}$, and $G_{n-1}, Q_{n-1} \in \mathbb{G}_{n-1}$ such that

$$G_{n-1}^T G_{n-2}^T \begin{bmatrix} 0 & 0 \\ 0 & M_2 \end{bmatrix} Z_{n-2} Q_{n-1} = \psi e_n e_n^T.$$

Using the orthogonal symplectic property,

$$G_{n-1}^T G_{n-2}^T \begin{bmatrix} I & 0 \\ 0 & M_1 \end{bmatrix} Z_{n-2} Q_{n-1} = \begin{bmatrix} I & 0 & 0 \\ 0 & \tilde{M}_1 & 0 \\ 0 & 0 & \phi \end{bmatrix},$$

where $\tilde{M}_1$ is 2×2 real orthogonal and $\phi^2 + \psi^2 = 1$. Note that we can choose the Givens rotations so that the sign of ϕ is the same as the sign of the determinant of M_1. Then $\tilde{M}_1$ is a Givens rotation, and

$$\tilde{G}_{n-2} = \begin{bmatrix} I & 0 & 0 \\ 0 & \tilde{M}_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \in \mathbb{G}_{n-2}.$$

Now, for

$$\mathcal{G}_{n-2} = \begin{bmatrix} G_{n-2} & 0 \\ 0 & G_{n-2} \end{bmatrix}, \quad \mathcal{G}_{n-1} = \begin{bmatrix} G_{n-1} & 0 \\ 0 & G_{n-1} \end{bmatrix}, \quad \tilde{\mathcal{G}}_{n-2} = \begin{bmatrix} \tilde{G}_{n-2} & 0 \\ 0 & \tilde{G}_{n-2} \end{bmatrix},$$

$$\mathcal{Q}_{n-1} = \begin{bmatrix} Q_{n-1} & 0 \\ 0 & Q_{n-1} \end{bmatrix}, \quad \mathcal{Z}_{n-2} = \begin{bmatrix} Z_{n-2} & 0 \\ 0 & Z_{n-2} \end{bmatrix},$$

and $\Gamma_n := \Gamma_n(\phi, \psi) \in \mathbb{SG}_n$, one has

$$\mathcal{M} = \mathcal{G}_{n-2}\mathcal{G}_{n-1}\tilde{\mathcal{G}}_{n-2}\Gamma_n \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T.$$

Therefore,

$$\Theta^T \mathcal{Y}^T \mathcal{S} \mathcal{Y} \Theta = \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-3}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\tilde{\mathcal{G}}_{n-2}\Gamma_n \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T.$$

We now start the third transformation with $\mathcal{Z}$. First,

$$\begin{aligned} \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T \Theta^T \mathcal{Y}^T \mathcal{S} \mathcal{Y} \Theta \mathcal{Z}_{n-2}\mathcal{Q}_{n-1} &= \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-4}\mathcal{G}_{n-3}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\tilde{\mathcal{G}}_{n-2}\Gamma_n \\ &=: \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-4}\tilde{\mathcal{Q}}_{n-1}\tilde{\mathcal{Z}}_{n-2}\mathcal{G}_{n-3}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\tilde{\mathcal{G}}_{n-2}\Gamma_n \end{aligned}$$

for some $\tilde{\mathcal{Q}}_{n-1} \in \mathbb{SG}_{n-1}$ and $\tilde{\mathcal{Z}}_{n-2} \in \mathbb{SG}_{n-2}$ so that $\mathcal{T} := \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T \mathcal{T} \tilde{\mathcal{Z}}_{n-2}^T \tilde{\mathcal{Q}}_{n-1}^T$ is symplectic upper triangular. For the product $\tilde{\mathcal{Q}}_{n-1}\tilde{\mathcal{Z}}_{n-2}\mathcal{G}_{n-3}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\tilde{\mathcal{G}}_{n-2}$ we perform the following turnovers:

$$\begin{aligned} &(n-1, \mathbf{n-2}, \mathbf{n-3}, \mathbf{n-2}, n-1, n-2) \to (\mathbf{n-1}, \mathbf{n-3}, n-2, \mathbf{n-3}, \mathbf{n-1}, n-2) \\ &= (n-3, \mathbf{n-1}, \mathbf{n-2}, \mathbf{n-1}, n-3, n-2) \to (n-3, n-2, n-1, \mathbf{n-2}, \mathbf{n-3}, \mathbf{n-2}) \\ &\to (n-3, n-2, \mathbf{n-1}, \mathbf{n-3}, n-2, n-3) = (n-3, n-2, n-3, n-1, n-2, n-3). \end{aligned}$$

We have

$$\begin{aligned} \mathcal{Q}_{n-1}^T \mathcal{Z}_{n-2}^T \Theta^T \mathcal{Y}^T \mathcal{S} \mathcal{Y} \Theta \mathcal{Z}_{n-2}\mathcal{Q}_{n-1} &=: \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-2}\tilde{\mathcal{G}}_{n-3}\mathcal{G}_{n-1}\mathcal{Q}_{n-2}^T \mathcal{Z}_{n-3}^T \Gamma_n \\ &= \mathcal{T}\mathcal{G}_1 \dots \mathcal{G}_{n-2}\tilde{\mathcal{G}}_{n-3}\mathcal{G}_{n-1}\Gamma_n \mathcal{Q}_{n-2}^T \mathcal{Z}_{n-3}^T. \end{aligned}$$

Similarly,

$$\begin{aligned}&\mathcal{Q}_{n-2}^T\mathcal{Z}_{n-3}^T\mathcal{Q}_{n-1}^T\mathcal{Z}_{n-2}^T\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta\mathcal{Z}_{n-2}\mathcal{Q}_{n-1}\mathcal{Z}_{n-3}\mathcal{Q}_{n-2}\\&\qquad=:\mathcal{T}\mathcal{G}_1\dots\mathcal{G}_{n-5}\tilde{\mathcal{Q}}_{n-2}\tilde{\mathcal{Z}}_{n-3}\mathcal{G}_{n-4}\mathcal{G}_{n-3}\mathcal{G}_{n-2}\tilde{\mathcal{G}}_{n-3}\mathcal{G}_{n-1}\Gamma_n\\&\qquad=:\mathcal{T}\mathcal{G}_1\dots\mathcal{G}_{n-4}\mathcal{G}_{n-3}\tilde{\mathcal{G}}_{n-4}\mathcal{G}_{n-2}\mathcal{G}_{n-1}\Gamma_n\mathcal{Q}_{n-3}^T\mathcal{Z}_{n-4}^T.\end{aligned}$$

Continuing the procedure, one arrives at

$$\mathcal{Q}_3^T\mathcal{Z}_2^T\dots\mathcal{Z}_{n-2}^T\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta\mathcal{Z}_{n-2}\dots\mathcal{Z}_2\mathcal{Q}_3=:\mathcal{T}\mathcal{G}_1\mathcal{G}_2\tilde{\mathcal{G}}_1\mathcal{G}_3\dots\mathcal{G}_{n-1}\Gamma_n\mathcal{Q}_2^T\mathcal{Z}_1^T.$$

Then

$$\begin{aligned}&\mathcal{Q}_2^T\mathcal{Z}_1^T\mathcal{Q}_3^T\mathcal{Z}_2^T\dots\mathcal{Q}_{n-1}^T\mathcal{Z}_{n-2}^T\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta\mathcal{Z}_{n-2}\mathcal{Q}_{n-1}\dots\mathcal{Z}_2\mathcal{Q}_3\mathcal{Z}_1\mathcal{Q}_2\\&\qquad=\mathcal{Q}_2^T\mathcal{Z}_1^T\mathcal{T}\mathcal{G}_1\mathcal{G}_2\tilde{\mathcal{G}}_1\mathcal{G}_3\dots\mathcal{G}_{n-1}\Gamma_n=:\mathcal{T}\tilde{\mathcal{Q}}_2\tilde{\mathcal{Z}}_1\mathcal{G}_1\mathcal{G}_2\tilde{\mathcal{G}}_1\mathcal{G}_3\dots\mathcal{G}_{n-1}\Gamma_n.\end{aligned}$$

Performing the following turnovers on $\tilde{\mathcal{Q}}_2\tilde{\mathcal{Z}}_1\mathcal{G}_1\mathcal{G}_2\tilde{\mathcal{G}}_1$,

$$(2,\mathbf{1},\mathbf{1},2,1)=:(\mathbf{2},\mathbf{1},\mathbf{2},1)\to(1,2,\mathbf{1},\mathbf{1})=:(1,2,1),$$

one has

$$\mathcal{Q}_2^T\mathcal{Z}_1^T\dots\mathcal{Q}_{n-1}^T\mathcal{Z}_{n-2}^T\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta\mathcal{Z}_{n-2}\mathcal{Q}_{n-1}\dots\mathcal{Z}_1\mathcal{Q}_2=:\mathcal{T}\tilde{\mathcal{G}}_1\mathcal{G}_2\mathcal{G}_3\dots\mathcal{G}_{n-1}\Gamma_n\mathcal{Q}_1^T.$$

Finally, let $\mathcal{Z}=\mathcal{Z}_{n-2}\mathcal{Q}_{n-1}\mathcal{Z}_{n-3}\mathcal{Q}_{n-2}\dots\mathcal{Z}_2\mathcal{Q}_3\mathcal{Z}_1\mathcal{Q}_2\mathcal{Q}_1$. One has

$$\begin{aligned}\mathcal{Z}^T\Theta^T\mathcal{Y}^T\mathcal{S}\mathcal{Y}\Theta\mathcal{Z}&=\mathcal{Q}_1^T\mathcal{T}\tilde{\mathcal{G}}_1\mathcal{G}_2\mathcal{G}_3\dots\mathcal{G}_{n-1}\Gamma_n\\&=:\mathcal{T}\tilde{\mathcal{Q}}_1\tilde{\mathcal{G}}_1\mathcal{G}_2\dots\mathcal{G}_{n-1}\Gamma_n=\mathcal{T}\mathcal{G}_1\mathcal{G}_2\dots\mathcal{G}_{n-1}\Gamma_n,\quad\mathcal{G}_1=\tilde{\mathcal{Q}}_1\tilde{\mathcal{G}}_1\in\mathbb{SG}_1,\end{aligned}$$

which completes one double shift symplectic QR iteration.

During the iteration process, as in the single shift case the Givens rotations $\tilde{Y}_1,\tilde{P}_2$, Y_i,P_{i+1}, for $i=2,\dots,n-2$, and the symplectic Givens rotations, $\tilde{\mathcal{Q}}_i,\tilde{\mathcal{Z}}_{i-1}$, for $i=n-1,\dots,2$, and $\tilde{\mathcal{Q}}_1$ can be determined from the entries from either T_{11} or T_{22}. The same strategy can be applied for improving numerical stability. Also, as in the single shift case, caution needs to be taken for determining the orthogonal symplectic matrices in Θ. In the discussions above we consider the exact symplectic situation and some entries will be automatically zero. In practice, setting these entries to zero may potentially introduce large errors.

The shifts σ_1,σ_2 can be selected to be the eigenvalues of the 2×2 leading principal submatrix of $\mathcal{S}$, i.e., $t^2-\mu t+\nu$ be the characteristic polynomial of this 2×2 submatrix. The stopping criterion is similar to the single shift case.

Finally, two economic versions corresponding to the double shift iterations can be developed.

4. Symplectic pairs. Consider the symplectic matrix pair $(\mathcal{A},\mathcal{B})$ with $\mathcal{A},\mathcal{B}\in\mathbb{C}^{2n\times2n}$, i.e., $\mathcal{A},\mathcal{B}$ satisfy $\mathcal{A}\mathcal{J}_n\mathcal{A}^*=\mathcal{B}\mathcal{J}_n\mathcal{B}^*$. Here we assume that at least $\mathcal{A}$ or $\mathcal{B}$ is invertible. For a more general symplectic pair, we may first perform an initial reduction process to deflate the singular part as well as the parts containing the eigenvalues zero and infinity. When $\mathcal{B}$ is invertible, $(\mathcal{A},\mathcal{B})$ is a symplectic pair if and only if $\mathcal{B}^{-1}\mathcal{A}$ is a symplectic matrix. We further assume that $\mathcal{B}^{-1}\mathcal{A}$ satisfies the rank condition (2.3). Note also that for any unitary matrix $\mathcal{X}$ and unitary symplectic matrix $\mathcal{Y}$, the transformation $(\mathcal{A},\mathcal{B})\to(\mathcal{X}\mathcal{A}\mathcal{Y},\mathcal{X}\mathcal{B}\mathcal{Y})$ preserves the symplectic structure.

A symplectic pair with all of the above assumptions can be initially reduced to a pair in the following factorized form with a unitary matrix $\mathcal{X}_0$ and a unitary symplectic matrix $\mathcal{V}_0$:

$$\mathcal{X}_0\mathcal{A}\mathcal{V}_0 = \mathcal{T}_1\mathcal{G}\Gamma_n, \quad \mathcal{X}_0\mathcal{B}\mathcal{V}_0 = \mathcal{T}_2, \quad \mathcal{G} = \mathcal{G}_1 \dots \mathcal{G}_{n-1}, \tag{4.1}$$

where $\mathcal{T}_1, \mathcal{T}_2$ are both skew upper triangular, $\mathcal{G}_i \in \mathbb{SG}_i$, $i = 1, \dots, n-1$, are symplectic Givens rotations and $\Gamma_n \in \mathbb{SG}_n$. Clearly, $\mathcal{V}_0^*(\mathcal{B}^{-1}\mathcal{A})\mathcal{V}_0$ is exactly in the form (3.1) with $\mathcal{T} := \mathcal{T}_2^{-1}\mathcal{T}_1$.

The process for computing (4.1) is similar to the triangular-Hessenberg reduction for a general pair in the QZ algorithm. We begin with a unitary matrix $\mathcal{X}_0$ such that

$$\mathcal{X}_0\mathcal{B} = \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix}, \quad B_{ij} \in \mathbb{C}^{n\times n}$$

is skew upper triangular. We partition

$$\mathcal{X}_0\mathcal{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

accordingly. By assumption, A_{21} is rank one. So it can be expressed as $A_{21} = fg^*$ for some column vectors $f, g \neq 0$. For g, we have Givens rotations $V_i \in \mathbb{G}_i$, $i = 1, \dots, n-1$, so that $V_{n-1}^* \dots V_1^* g = \alpha e_n$. For each V_i, one can determine Givens rotations $\tilde{X}_i, X_i \in \mathbb{G}_i$ such that $B_{11} := \tilde{X}_i B_{11} V_i$ stays upper triangular and $B_{22} := X_i B_{22} V_i$ stays lower triangular. Then for

$$\tilde{\mathcal{X}}_0 := \begin{bmatrix} \tilde{X}_{n-1} & 0 \\ 0 & X_{n-1} \end{bmatrix} \dots \begin{bmatrix} \tilde{X}_1 & 0 \\ 0 & X_1 \end{bmatrix}, \quad \mathcal{V}_0 = \begin{bmatrix} V_1 & 0 \\ 0 & V_1 \end{bmatrix} \dots \begin{bmatrix} V_{n-1} & 0 \\ 0 & V_{n-1} \end{bmatrix},$$

$f := \bar{\alpha}\tilde{\mathcal{X}}_0 f$, and $\mathcal{X}_0 := \tilde{\mathcal{X}}_0\mathcal{X}_0$, one has

$$\mathcal{X}_0\mathcal{A}\mathcal{V}_0 =: \begin{bmatrix} A_{11} & A_{12} \\ fe_n^* & A_{22} \end{bmatrix}, \quad \mathcal{X}_0\mathcal{B}\mathcal{V}_0 =: \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix},$$

where $\mathcal{X}_0\mathcal{B}\mathcal{V}_0$ is still skew upper triangular. Similar to the matrix case, the symplectic property implies that $A_{22}e_n$ is parallel to f and there is a symplectic unitary matrix $\Gamma_n \in \mathbb{SG}_n$ such that

$$\mathcal{X}_0\mathcal{A}\mathcal{V}_0\Gamma_n^T =: \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}.$$

The rest of the reductions are just like the triangular-Hessenberg reductions on the pair (A_{11}, B_{11}), or equivalently, (A_{22}, B_{22}), by using $A_{22}A_{11}^* = B_{22}B_{11}^*$, which is from the fact that the current matrix pair is still symplectic. We determine $V_i \in \mathbb{G}_i$, $i = 1, \dots, n-2$, and $G_{n-1} \in \mathbb{G}_{n-1}$ so that the last row of $A_{11}V_1 \dots V_{n-2}G_{n-1}^*$ is in $\operatorname{span}\{e_n^*\}$. For each V_i, $i \in \{1, \dots, n-2\}$, one has $\tilde{X}_i \in \mathbb{G}_i$ and $X_i \in \mathbb{G}_i$ so that $B_{11} := \tilde{X}_i B_{11} V_i$ stays upper triangular and $B_{22} := X_i B_{22} V_i$ stays lower triangular. Define

$$\mathcal{G}_{n-1} = \begin{bmatrix} G_{n-1} & 0 \\ 0 & G_{n-1} \end{bmatrix},$$

and

$$\mathcal{X}_0 := \begin{bmatrix} \tilde{X}_{n-2} & 0 \\ 0 & X_{n-2} \end{bmatrix} \dots \begin{bmatrix} \tilde{X}_1 & 0 \\ 0 & X_1 \end{bmatrix} \mathcal{X}_0,$$
$$\mathcal{V}_0 := \mathcal{V}_0 \begin{bmatrix} V_1 & 0 \\ 0 & V_1 \end{bmatrix} \dots \begin{bmatrix} V_{n-2} & 0 \\ 0 & V_{n-2} \end{bmatrix}.$$

Because Γ_n commutes with

$$\begin{bmatrix} V_i & 0 \\ 0 & V_i \end{bmatrix} (i = 1, \dots, n-2),$$

one has

$$\mathcal{X}_0 \mathcal{A} \mathcal{V}_0 \Gamma_n^T \mathcal{G}_{n-1}^* =: \left[\begin{array}{cc|cc} * & * & * & * \\ 0 & * & * & * \\ \hline 0 & 0 & * & 0 \\ 0 & 0 & * & * \end{array}\right], \qquad \mathcal{X}_0 \mathcal{B} \mathcal{V}_0 =: \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix},$$

and $\mathcal{X}_0 \mathcal{B} \mathcal{V}_0$ is still skew upper triangular. We continue the process and eventually one has

$$\mathcal{X}_0 \mathcal{A} \mathcal{V}_0 \Gamma_n^T \mathcal{G}_{n-1}^* \dots \mathcal{G}_1^* = \mathcal{T}_1, \quad \mathcal{X}_0 \mathcal{B} \mathcal{V}_0 = \mathcal{T}_2,$$

which leads to the factored form (4.1).

Both the single and double shift QZ iterations can be constructed in a way similar to the symplectic matrix case. The only difference is that the updates of $\mathcal{T}$ are changed to that of $\mathcal{T}_2^{-1}\mathcal{T}_1$, which are simply generalized to

$$\mathcal{T} := \mathcal{G}_i^* \mathcal{T} \tilde{\mathcal{G}}_i \quad \to \quad \mathcal{T}_1 := \mathcal{X}_i \mathcal{T}_1 \tilde{\mathcal{G}}_i, \quad \mathcal{T}_2 := \mathcal{X}_i \mathcal{T}_2 \mathcal{G}_i$$

and

$$\mathcal{T} := \Delta \mathcal{T}_i \tilde{\Delta} \quad \to \quad \mathcal{T}_1 := \Phi \mathcal{T}_1 \tilde{\Delta}, \quad \mathcal{T}_2 := \Phi \mathcal{T}_2 \Delta,$$

where $\mathcal{G}_i, \tilde{\mathcal{G}}_i \in \mathbb{SG}_i$,

$$\mathcal{X}_i = \begin{bmatrix} \tilde{X}_i & 0 \\ 0 & X_i \end{bmatrix}$$

with $\tilde{X}_i, X_i \in \mathbb{G}_i$, $\Delta, \tilde{\Delta} \in \mathbb{SG}_n$, and $\Phi \in \mathbb{G}_{n,2n}$.

For a general symplectic pair, it might be a good idea to perform the transformations on full matrices. Economic versions of the algorithm may be considered in some special cases. For instance, a symplectic matrix pair arising from systems and control commonly has the particular form

$$\left(\begin{bmatrix} F & 0 \\ H & I \end{bmatrix}, \begin{bmatrix} I & -C \\ 0 & F^* \end{bmatrix} \right), \quad H = H^*, \quad C = C^*, \quad \operatorname{rank} H = 1, \quad \det F \neq 0.$$

If the above initial reduction process is applied to this pair, it may not be able to take advantage of the additional structures. However, such a pair may be reduced to the factored form (3.1) directly by working on the symplectic matrix

$$\mathcal{S} = \begin{bmatrix} I & -C \\ 0 & F^* \end{bmatrix}^{-1} \begin{bmatrix} F & 0 \\ H & I \end{bmatrix} = \begin{bmatrix} I & C \\ 0 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & F^{-*} \end{bmatrix} \begin{bmatrix} I & 0 \\ H & I \end{bmatrix}.$$

Clearly, there is a unitary matrix V_0 such that $V_0^* H V_0 = b e_n e_n^T$ with $b \in \mathbb{R}$. Let $C := V_0^* C V_0$ and $F := V_0^* F V_0$. For

$$\mathcal{V}_0 = \begin{bmatrix} V_0 & 0 \\ 0 & V_0 \end{bmatrix},$$

one has

$$\mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 =: \begin{bmatrix} I & C \\ 0 & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & F^{-*} \end{bmatrix} \begin{bmatrix} I & 0 \\ b e_n e_n^T & I \end{bmatrix}.$$

For $\Gamma_n = \Gamma_n(\phi, \psi)$ with $\phi = 1/r, \psi = -b/r$, and $r = \sqrt{1+b^2}$, one has

$$\begin{bmatrix} I & 0 \\ be_n e_n^T & I \end{bmatrix} = \left[\begin{array}{cc|cc} I & & 0 & \\ & r^{-1} & & r^{-1}b \\ \hline & & I & \\ & & & r \end{array}\right] \Gamma_n.$$

Then, we have

$$\mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 = \begin{bmatrix} I & C \\ 0 & I \end{bmatrix} \begin{bmatrix} \hat{F} & br^{-1} f_n e_n^T \\ 0 & \hat{F}^{-*} \end{bmatrix} \Gamma_n = \begin{bmatrix} \hat{F} & \hat{W}\hat{F}^{-*} \\ 0 & \hat{F}^{-*} \end{bmatrix} \Gamma_n,$$

where

$$\hat{F} = F \begin{bmatrix} I & 0 \\ 0 & r^{-1} \end{bmatrix},$$

$f_n = Fe_n$, and $\hat{W} = C + \frac{b}{r^2} f_n f_n^*$. Applying a Hessenberg reduction process to $\hat{F}$, we can determine a unitary matrix V_1 with $V_1 e_n = e_n$, an upper triangular matrix T_{11}, and Givens rotations $G_1, \ldots, G_{n-1}$ such that $V_1^* \hat{F} V_1 = T_{11} G_1 \ldots G_{n-1} =: T_{11} G$. Let

$$\mathcal{V}_0 := \mathcal{V}_0 \begin{bmatrix} V_1 & 0 \\ 0 & V_1 \end{bmatrix}, \quad W = V_1^* \hat{W} V_1, \quad \mathcal{G} = \begin{bmatrix} G & 0 \\ 0 & G \end{bmatrix}, \text{ and } \mathcal{T} = \begin{bmatrix} T_{11} & WT_{11}^{-*} \\ 0 & T_{11}^{-*} \end{bmatrix},$$

one has $\mathcal{V}_0^* \mathcal{S} \mathcal{V}_0 = \mathcal{T}\mathcal{G}\Gamma_n$, and the second economic version of the core-chasing symplectic QR algorithm may apply to this form to update T_{11} and W only.

5. Conclusions.

We proposed an improved version of the symplectic QR algorithm [20] for solving the eigenvalue problem of symplectic matrices with a rank condition. For symplectic matrices, the algorithm is based on a factored form of a symplectic upper Hessenberg matrix that further exploits the symplectic structure, so that a core-chasing symplectic QR iteration is able to be developed. The proposed algorithm is more numerically stable than the method in [20], Still, backward stability cannot be established due to the fact that the initial symplectic upper Hessenberg reduction process may not necessarily be numerically backward stable. Two economic versions of the algorithm are also proposed to take use of the symplectic structure even more efficiently. However, they may be less numerically stable. Numerical results show that the algorithm works well in practice. For symplectic pairs, a generalized version of the algorithm can be constructed.

It seems that it is still a fundamentally challenging problem for developing a symplectic eigenvalue algorithm that is both numerically backward stable and strictly structure preserving. Further research needs to be done to address this issue.

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REFERENCES

[1] J. L. Aurentz, T. Mach, L. Robol, R. Vandebril, and D. S. Watkins, *Core-Chasing Algorithms for Eigenvalue Problem*, Fundamentals of Algorithms 13, SIAM, Philadelphia, 2018, https://doi.org/10.1137/1.9781611975345.

[2] P. Benner and H. Fassbender, *The symplectic eigenvalue problem, the butterfly form, the SR algorithm, and the Lanczos method*, Linear Algebra Appl., 275/276 (1998), pp. 19–47.

[3] P. Benner, H. Fassbender, and D. S. Watkins, *SR and SZ algorithms for the symplectic (butterfly) eigenproblem*, Linear Algebra Appl., 287(1999), pp. 41–76.

[4] P. Benner, A. Laub, and V. Mehrmann, *A collection of benchmark examples for the numerical solution of algebraic Riccati equations II: Discrete-time case*, Technical Report SPC 95-23, Fak. f. Mathematik TU Chemnitz-Zwickau, 09107 Chemnitz, FRG, 1995, J. Comput. Appl. Math., 86 (1997), pp. 17–43.

[5] P. Benner, V. Mehrmann, and H. Xu, *A new method for computing the stable invariant subspace of a real Hamiltonian matrix*, J. Comput. Appl. Math., 86 (1997), pp. 17–43.

[6] P. Benner, V. Mehrmann, and H. Xu, *A numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian or symplectic pencils*, Numer. Math., 78 (1998), pp. 329–358.

[7] P. Benner, V. Mehrmann, and H. Xu, *A note on the numerical solution of complex Hamiltonian and skew-Hamiltonian eigenvalue problems*, Electron. Trans. Numer. Anal., 8 (1999), pp. 115–126.

[8] A. Bunse-Gerstner, *Symplectic QR-like algorithms*, Habilitationsschrift, Universitit Bielefeld, Bielefeld Germany, 1986.

[9] A. Bunse-Gerstner and V. Mehrmann, *A symplectic QR-like algorithm for the solution of the real algebraic Riccati equation*, IEEE Trans. Automat. Control, 31 (1986), pp. 1104–1113.

[10] R. Byers, *Hamiltonian and Symplectic Algorithms for the Algebraic Riccati Equation*, Ph.D. thesis, Cornell University, Ithaca, NY, 1983.

[11] R. Byers, *A Hamiltonian QR-algorithm*, SIAM J. Sci. and Stat. Comput., 7 (1986), pp. 212–229, https://doi.org/10.1137/0907015.

[12] D. Chu, X. Liu, and V. Mehrmann, *A numerical method for computing the Hamiltonian Schur form*, Numer. Math., 105 (2007), pp. 375–412.

[13] H. Fassbender, *Symplectic Methods for the Symplectic Eigenproblem*, Kluwer Academic/Plenum, New York, 2000.

[14] H. Fassbender, *The parameterized SR algorithm for symplectic (butterfly) matrices*, Math. Comput., 70 (2001), pp. 1515–1541.

[15] H. Fassbender and D. Kressner, *Structured eigenvalue problems*, GAMM-Mitt., 29 (2006), pp. 297–318.

[16] U. Flaschka, V. Mehrmann, and D. Zywietz, *An analysis of structure preserving numerical methods for symplectic eigenvalue problems*, RAIRO Automat.-Prod. Inform. Ind., 25 (1991), pp. 165–189.

[17] P. Lancaster and L. Rodman, *The Algebraic Ricccati Equation*. Oxford University Press, Oxford, 1995.

[18] B. C. Levy, R. Frezza, and A. J. Krener, *Modeling and estimation of discrete-time Gaussian reciprocal processes*, IEEE Trans. Automat. Control, 35 (1990), pp. 1013–1023.

[19] W.-W. Lin, V. Mehrmann, and H. Xu, *Canonical forms for Hamiltonian and symplectic matrices and pencils*, Linear Algebra Appl., 302/303 (1999), pp. 469–533.

[20] V. Mehrmann, *A symplectic orthogonal method for single input or single output discrete time optimal quadratic control problems*, SIAM J. Matrix Anal. Appl., 9 (1988), pp. 221–247, https://doi.org/10.1137/0609019.

[21] V. Mehrmann, *The Autonomous Linear Quadratic Control Problem, Theory and Numerical Solution*, Lect. Notes Control Inf. Sci. 163, Springer-Verlag, Heidelberg, 1991.

[22] T. Pappas, A. J. Laub, and N. R. Sandell, *On the numerical solution of the discrete-time algebraic Riccati equation*, IEEE Trans. Automat. Control., 25 (1980), pp. 631–641.

[23] R. Vandebril, *Chasing bulges or rotations? A metamorphosis of the QR-algorithm*, SIAM J. Matrix Anal. Appl., 32 (2011), pp. 217–247, https://doi.org/10.1137/100809167.

[24] R. Vandebril and D. S. Watkins, *A generalization of the multishift QR algorithm*, SIAM J. Matrix Anal. Appl., 33 (2012), pp. 759–779, https://doi.org/10.1137/11085219X.