

On Hamiltonian and Symplectic Hessenberg Forms*

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ABSTRACT

Characterizations are given for the Hamiltonian matrices that can be reduced to Hamiltonian Hessenberg form and the symplectic matrices that can be reduced to symplectic Hessenberg form by orthogonal symplectic similarity transformations. The reduction to these special Hessenberg forms is the missing link in the solution of the open problem of constructing a stable structure-preserving QR-like method of complexity $O(n^3)$ for the computation of invariant subspaces of Hamiltonian and symplectic matrices. Our considerations lead us to propose an approach to the computation of Lagrangian invariant subspaces of a Hamiltonian or symplectic matrix.

1. INTRODUCTION

The numerical computation of invariant subspaces of a matrix A is usually performed via a similarity transformation of A to a triangular-like

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form. For example, if $A \in \mathbb{R}^{n,n}$, an appropriate triangular-like form is the *real Schur form* (also called *upper quasitriangular form*), in which the matrix is upper triangular except for possible 2×2 blocks on the diagonal that correspond to complex conjugate eigenvalues. The numerically stable computation of this form can be obtained using the *QR* algorithm, which performs a sequence of unitary similarity transformations on the original matrix A . The reduction of the initial matrix A to Hessenberg form is essential for the use of the *QR* algorithm for several reasons, including the fact that the Hessenberg form provides a condensed form that is invariant under the *QR* iteration. This enables the *QR* iteration to be performed using $O(n^2)$ arithmetic operations per step. Another important fact is that any square matrix can be reduced to Hessenberg form in a finite number of steps, using $O(n^3)$ operations, so the reduction to Hessenberg form is defined for all matrices A .

The computation of invariant subspaces of Hamiltonian or symplectic matrices is an important task in many applications, such as linear-quadratic optimal control or the solution of algebraic Riccati equations. See, e.g., [4, 10, 13, 14, 17, 22]. Consequently, research has been focused on the development of efficient, numerically reliable algorithms for these eigenproblems that take advantage of the Hamiltonian or symplectic structure.

DEFINITION 1.1. Let

$$J := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix},$$

where I_n is the $n \times n$ identity matrix. Then we say that

- (1) $A \in \mathbb{R}^{2n,2n}$ is *symplectic* if $A^T J A = J$;
- (2) $A \in \mathbb{R}^{2n,2n}$ is *Hamiltonian* if $(AJ)^T = -AJ$.

Structure-preserving methods for computing eigenvalues and invariant subspaces of Hamiltonian and symplectic matrices are based on the fact that symplectic similarity transformations preserve Hamiltonian and symplectic structure. Triangular-like forms for Hamiltonian and symplectic matrices are for example discussed in [5, 6, 15, 17, 18, 20, 21]. Hessenberg-like forms and *QR*-type algorithms for Hamiltonian and symplectic matrices have also been introduced; see, e.g., [4–6, 18]. We summarize the Hessenberg and Schur forms for Hamiltonian and symplectic matrices below.

DEFINITION 1.2.

(i) Let $A = [a_{ij}] \in \mathbb{R}^{2n, 2n}$ be Hamiltonian; then

(1) A is in *Hamiltonian Hessenberg form* if

$$(1.3) \quad A = \begin{bmatrix} F & G \\ H & -F^T \end{bmatrix} \triangleq \begin{bmatrix} \square & \square \\ * & \square \end{bmatrix},$$

i.e., $F = [f_{ij}] \in \mathbb{R}^{n, n}$ is an upper Hessenberg matrix, $H = \alpha e_n e_n^T$, where e_n is the n th unit vector, and G is symmetric;

(2) The Hamiltonian Hessenberg matrix A is called *unreduced* if

$$f_{i+1, i} \neq 0, \quad i = 1, \dots, n-1, \quad \text{and} \quad \alpha \neq 0;$$

(3) A is in *real Hamiltonian Schur form* if

$$(1.4) \quad A = \begin{bmatrix} T & R \\ 0 & -T^T \end{bmatrix},$$

where T is in real Schur form and R is symmetric.

(ii) Let $A = [a_{ij}] \in \mathbb{R}^{2n, 2n}$ be symplectic; then

(1) A is in *symplectic Hessenberg form* if

$$(1.5) \quad A = [a_{ij}] = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \triangleq \begin{bmatrix} \square & \square \\ 0 \mid \square \end{bmatrix},$$

where A_{11} is an upper Hessenberg matrix and $A_{21} = e_n u^T$ for $u \in \mathbb{R}^n$.

(2) The symplectic Hessenberg matrix A is called *unreduced* if

$$a_{i+1, i} \neq 0, \quad i = 1, \dots, n-1, \quad \text{and} \quad a_{2n, n} \neq 0.$$

(3) The symplectic matrix A is said to be in *symplectic Schur form* if

$$(1.6) \quad A = \begin{bmatrix} T & R \\ 0 & T^{-T} \end{bmatrix},$$

where T is in real Schur form.

QR -type algorithms for Hamiltonian and symplectic matrices that arise in single-input or single-output linear regulator problems are presented in [5] and [18]. These methods use only orthogonal symplectic similarity transformations, require $O(n^3)$ arithmetic operations, and are strongly stable in the sense of [2]. In these cases the initial matrix is first transformed to Hamiltonian or symplectic Hessenberg form using finitely many steps. This form then stays invariant under the QR -like iteration. In the general case, however, the efficient, numerically stable computation of the Hamiltonian or symplectic Schur form with a method that uses only orthogonal symplectic similarity transformations remains an open problem. The major obstacle in the development of such an algorithm is the reduction of a general Hamiltonian or symplectic matrix to the appropriate Hessenberg-like form.

In Section 2 we consider the reduction of a Hamiltonian or symplectic matrix A to its Hessenberg-like form $Q^T A Q$, where Q is orthogonal and symplectic, in terms of an Arnoldi process. We will see that the components of the first column of Q must satisfy a system of n quadratic equations in $2n$ unknowns. Consequently, such a reduction is not always possible. Moreover, we show that if the Hessenberg-like matrix $Q^T A Q$ is unreduced, the transformation matrix Q is essentially determined by its first column. These considerations provide insight into the reasons that the problem of reducing a general Hamiltonian or symplectic matrix to its Hessenberg-like form remains open.

The ideas of Section 2 lead us to propose an algorithm in Section 3 for the computation of Lagrangian invariant subspace of a Hamiltonian or symplectic matrix.

DEFINITION 1.7. A subspace \mathcal{D} of \mathbb{R}^{2n} is called *isotropic* if $x^T J y = 0$ for all $x, y \in \mathcal{D}$. A *Lagrangian* subspace is a maximal isotropic subspace (i.e., an isotropic subspace that is not contained in a larger isotropic subspace).

Note that Lagrangian subspaces of \mathbb{R}^{2n} are of dimension n .

It is easily seen that if λ is an eigenvalue of a real Hamiltonian matrix, then so is $-\lambda$. Similarly, if λ is an eigenvalue of a real symplectic matrix, then so is $1/\lambda$. (See, e.g., [15, 20].) If a Hamiltonian matrix has no purely imaginary eigenvalue, we refer to the eigenspace corresponding to the

eigenvalues with negative real part as the *stable* invariant subspace of A . If a symplectic matrix A has no eigenvalue of unit modulus, the eigenspace corresponding to eigenvalues with moduli less than one is the *stable* invariant subspace of A . The computation of the stable invariant subspace of such a Hamiltonian or symplectic matrix is of importance in the solution of the algebraic Riccati equations that arise in linear control theory. (See [12] and the references therein.) Observe that the stable invariant subspace of a Hamiltonian or symplectic matrix is necessarily Lagrangian. The proposed method can therefore be used in the construction of the solution of the algebraic Riccati equations of control theory.

2. MAIN RESULTS

It is observed in [6] that a Hamiltonian matrix A is in Hamiltonian Hessenberg form if and only if $P^{-1}AP$ is in the usual Hessenberg form

$$\begin{bmatrix} \diagdown & & \\ & \diagdown & \\ & & \diagdown \end{bmatrix},$$

where

$$P = P^{-1} = \begin{bmatrix} I & & 0 & & \\ & & & & 1 \\ 0 & & & \ddots & \\ & & 1 & & \\ & & & & \end{bmatrix}.$$

Consequently, a version of the implicit Q theorem (see [9, p. 367]) holds for Hamiltonian Hessenberg matrices; that is, an orthogonal matrix that transforms A to unreduced Hamiltonian Hessenberg form is essentially determined by its first column. An analogous result holds for the reduction of a symplectic matrix to symplectic Hessenberg form. In particular, we have the following result.

PROPOSITION 2.1.

(i) *Let $A \in \mathbb{R}^{2n, 2n}$ be Hamiltonian, and let $U, V \in \mathbb{R}^{2n, 2n}$ be orthogonal symplectic matrices such that*

$$(2.2) \quad A_1 = U^T A U, \quad A_2 = V^T A V$$

are in unreduced Hamiltonian Hessenberg form. Let u_j and v_j denote the j th columns of U and V , respectively, and assume that $u_1 = v_1$. Further assume that the elements of A_1 and A_2 in positions $(i+1, i)$, $i = 1, \dots, n-1$, and $(2n, n)$ are positive. Then $u_j = v_j$ for each $j = 2, \dots, 2n$ and $A_1 = A_2$.

(ii) Let $A \in \mathbb{R}^{2n, 2n}$ be symplectic, and let $U, V \in \mathbb{R}^{2n, 2n}$ be orthogonal symplectic matrices such that

$$(2.3) \quad A_1 = U^T A U, \quad A_2 = V^T A V$$

are in unreduced symplectic Hessenberg form. Let u_j and v_j denote the j th columns of U and V , respectively, and assume that $u_1 = v_1$. Further assume that the elements of A_1 and A_2 in positions $(i+1, i)$, $i = 1, \dots, n-1$, and $(2n, n)$ are positive. Then $u_j = v_j$ for each $j = 2, \dots, 2n$ and $A_1 = A_2$.

Proof. (i): Clear by the above remarks, or see [6].

(ii): Since the first $n-1$ columns of a symplectic Hessenberg matrix are already those of a Hessenberg matrix, the implicit Q theorem implies that the first n columns of U and V in (2.3) are identical. The stated result then follows from the fact that any orthogonal symplectic matrix has the form

$$(2.4) \quad Q = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix},$$

and is therefore determined by its first n columns. This argument also applies to the proof of (i), since the first $n-1$ columns of a Hamiltonian Hessenberg matrix are also those of a matrix in the usual Hessenberg form. \blacksquare

Thus, the reduction to unreduced Hamiltonian or symplectic Hessenberg form, if it exists, is determined by the first column of the transformation matrix Q . If the first column of Q is given, the generation of the remaining columns of Q and the resulting reduction of the initial Hamiltonian or symplectic matrix can be performed using the following Arnoldi-type algorithm. We present this algorithm for theoretical purposes only; it may not be numerically reliable due to the divisions by possibly tiny subdiagonal elements and also due to the possible loss of orthogonality in the generated columns of Q caused by roundoff (see [24, p. 383]).

ALGORITHM 2.5. Let $A \in \mathbb{R}^{2n, 2n}$ be a Hamiltonian (or symplectic) matrix, and suppose that there exists an orthogonal and symplectic matrix

$Q \in \mathbb{R}^{2n, 2n}$ such that $\tilde{A} = Q^T A Q$ is in unreduced Hamiltonian (symplectic) Hessenberg form with positive elements in positions $(i + 1, i)$, $i = 1, \dots, n - 1$, and $(2n, n)$. Let $q_1 \in \mathbb{R}^{2n}$ be the first column of such a matrix Q . Then the following algorithm determines \tilde{A} and the remaining columns q_2, \dots, q_{2n} of Q .

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Set  $q_{n+1} = Jq_1$ .
FOR  $i = 1, n - 1$ 
    FOR  $j = 1, i$ 
         $\tilde{a}_{j,i} = q_j^T A q_i$ 
         $\tilde{a}_{n+j,i} = q_j^T J^T A q_i = 0$ 
    END FOR
     $\tilde{a}_{i+1,i} = \|(A - \tilde{a}_{ii}I)q_i - \sum_{j=1}^{i-1} q_j \tilde{a}_{ji}\|_2$ 
     $q_{i+1} = (1/\tilde{a}_{i+1,i})(A - \tilde{a}_{ii}I)q_i - \sum_{j=1}^{i-1} q_j \tilde{a}_{ji}$ 
     $q_{n+i+1} = Jq_{i+1}$ 
END FOR
FOR  $j = 1, n$ 
     $\tilde{a}_{j,n} = q_j^T A q_n$ 
     $\tilde{a}_{n+j,n} = q_j^T J^T A q_n$ 
END FOR
FOR  $i = 1, n$ 
    FOR  $j = 1, n$ 
         $\tilde{a}_{j,n+i} = q_j^T A q_{n+i}$ 
         $\tilde{a}_{n+j,n+i} = q_{n+j}^T A q_{n+i}$ 
    END FOR
END FOR
END
```

We now use Algorithm 2.5 to prove the following result.

THEOREM 2.6.

(i) *Let $A \in \mathbb{R}^{2n, 2n}$ be Hamiltonian. Then there exists an orthogonal and symplectic matrix $Q \in \mathbb{R}^{2n, 2n}$ such that $Q^T A Q$ is an unreduced Hamiltonian Hessenberg matrix if and only if the nonlinear system of equations*

$$(2.7) \quad \begin{aligned} x^T J A^{2i-1} x &= 0, & i = 1, \dots, n - 1, \\ x^T x &= 1 \end{aligned}$$

has a solution vector that is not contained in an invariant subspace of A of dimension less than or equal to n .

(ii) *Let $A \in \mathbb{R}^{2n, 2n}$ be symplectic. Then there exists an orthogonal and symplectic matrix $Q \in \mathbb{R}^{2n, 2n}$ such that $Q^T A Q$ is an unreduced symplectic*

$q_1^T q_1 = 1$, $q_1^T J q_1 = q_{n+1}^T J q_{n+1} = 0$, $q_{n+1}^T J q_1 = -q_1^T q_1 = -1$. Assume that we have shown that

$$(2.9) \quad \left. \begin{aligned} q_j^T q_k &= \delta_{jk} \\ q_j^T J q_k &= 0 \end{aligned} \right\} \quad \text{for } j, k \leq i,$$

where $i < n$. By Algorithm 2.5 we get

$$q_j^T q_{i+1} = \frac{1}{\tilde{a}_{i+1,i}} q_j^T (A - \tilde{a}_{ii} I) q_i - \sum_{l=1}^{i-1} q_j^T q_l \tilde{a}_{li}.$$

If $j \leq i$, then by the inductive assumption (2.9)

$$q_j^T q_{i+1} = \frac{1}{\tilde{a}_{i+1,i}} (\tilde{a}_{ji} - \tilde{a}_{ji}) = 0.$$

If $j = i + 1$, then

$$q_j^T q_{i+1} = q_{i+1}^T \Lambda q_i \frac{1}{\tilde{a}_{i+1,i}} = 1.$$

By the definition of $\tilde{a}_{i+1,i}$ we have

$$q_j^T J q_{i+1} = \frac{1}{\tilde{a}_{i+1,i}} \left(q_j^T J A q_i - \tilde{a}_{ii} q_j^T J q_i - \sum_{l=1}^{i-1} q_j^T J q_l \tilde{a}_{li} \right).$$

By applying the inductive assumption (2.9) and Algorithm 2.5 recursively, we get

$$(2.10) \quad q_j^T J q_{i+1} = q_1^T (A^{j-1})^T J A^i q_1 \frac{1}{\prod_{k=1}^i \tilde{a}_{k+1,k} \prod_{k=1}^{j-1} \tilde{a}_{k+1,k}}.$$

For even $i + j - 1$ (2.10) vanishes, since J is skew symmetric and $AJ = (JA)^T$. For odd $i + j - 1$ it vanishes by (2.7) (since $i + j - 1 \leq 2n - 2$). Thus, by induction, Q is orthogonal and symplectic.

(ii) \Rightarrow : Suppose that Q is orthogonal and symplectic such that $Z := Q^T A Q$ is an unreduced symplectic Hessenberg matrix of the form

$$\begin{bmatrix} \square & \square \\ 0 & \square \end{bmatrix}.$$

Then it is clear that q_1 is not in an invariant subspace of dimension less than or equal to n of A . Now $q_1^T J A^i q_1 = -e_{n+1}^T (Q^T A Q)^i e_1$. It follows trivially that the element in position $(n+1, 1)$ of Z^j vanishes for all powers $j = 1, \dots, n-1$. Thus (2.8) holds for $x = q_1$.

\Leftarrow : Proceeding as in part (i), we only have to show that

$$(2.11) \quad \left. \begin{array}{l} q_i^T q_j = \delta_{ij} \\ q_i^T J q_j = 0 \end{array} \right\} \quad \text{for } i = 1, \dots, n, \quad j \leq i.$$

The orthogonality of the q_i follows again by construction, while the second equality follows again inductively, using (2.10). Observe that since A is symplectic,

$$q_1^T (A^{j-1})^T J A^i q_1 = q_1^T J A^{i-j+1} q_1 = 0 \quad \text{by (2.8).} \quad \blacksquare$$

Note that if x satisfies the conditions (2.7) [or (2.8)] and is not contained in an invariant subspace of dimension n or less, then in the resulting reduction to the condensed form

$$\begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix}$$

for symplectic matrices as described in [3], or

$$\begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix}$$

for Hamiltonian matrices as described in [20], we obtain zeros in positions $(n + j, j)$, $j = 1, \dots, n - 1$. Thus, if the Hessenberg matrices in the upper left block are unreduced, then it follows by Proposition 2.1 that these condensed forms reduce to symplectic (or Hamiltonian) Hessenberg form. This observation explains why it is so difficult to obtain the symplectic (or Hamiltonian) Hessenberg form. Only if a correct first column for the orthogonal symplectic transformation matrix is chosen does one obtain these sufficiently reduced forms. (Also see [1].)

Observe also that Theorem 2.6 shows that a reduction to unreduced Hamiltonian or symplectic Hessenberg form does not always exist. For example, if A is Hamiltonian and JA is positive definite, then clearly no vector satisfying (2.7) exists. Similarly, if A is the symplectic matrix J^T , then (2.8) cannot be fulfilled. On the other hand, the Hamiltonian Schur form is a special case of the Hamiltonian Hessenberg form. Consequently, (2.7) is solvable if the Hamiltonian matrix A has no eigenvalue that is purely imaginary, since this condition guarantees the existence of the Hamiltonian Schur form (see, e.g., [20]). Similarly, (2.8) is solvable if the symplectic matrix A has no eigenvalue of unit modulus.

We do not know necessary and sufficient conditions for the existence of a vector satisfying (2.7) and (2.8) that is not contained in an invariant subspace of dimension less than or equal to n . An obvious necessary condition for the existence of a reduction to unreduced Hamiltonian or symplectic Hessenberg form is that A has no eigenvalue of geometric multiplicity larger than 1.

Sufficient conditions for the existence of such a vector satisfying (2.7) or (2.8) are given in the following proposition.

PROPOSITION 2.12.

(i) *Let $A \in \mathbb{R}^{2n, 2n}$ be a Hamiltonian matrix, and let \mathcal{D} be an isotropic A -invariant subspace of \mathbb{R}^{2n} . Then any $x \in \mathcal{D}$ with $\|x\|_2 = 1$ satisfies the conditions (2.7).*

(ii) *Let $A \in \mathbb{R}^{2n, 2n}$ be a symplectic matrix, and let \mathcal{D} be an isotropic A -invariant subspace of \mathbb{R}^{2n} . Then any $x \in \mathcal{D}$ such that $\|x\|_2 = 1$ satisfies the conditions (2.8).*

Proof. Since the subspace \mathcal{D} is A -invariant, it follows that $A^k x = y \in \mathcal{D}$ for any $k = 1, \dots, 2n$, and since \mathcal{D} is isotropic, it follows that $x^T J y = 0$. This proves (i) and (ii). ■

In particular it follows from Proposition 2.12 that any eigenvector satisfies the conditions (2.7) [or (2.8), respectively].

3. AN ALGORITHM FOR COMPUTING LAGRANGIAN INVARIANT SUBSPACES

A vector $x \in \mathbb{R}^{2n}$ satisfying the conditions of Proposition 2.12 is contained in an invariant subspace of dimension at most n , so it does not determine an unreduced Hamiltonian or symplectic Hessenberg matrix. But such a choice can be used to find the stable invariant subspace of a Hamiltonian or symplectic matrix, which is often the original problem one wishes to solve.

Van Loan [23] and Lin [16] proposed numerical methods to compute the eigenvalues of Hamiltonian and symplectic matrices, respectively, but not the corresponding invariant subspaces. The following result indicates how one can use these computed eigenvalues to determine the corresponding invariant subspaces.

PROPOSITION 3.1.

(i) *Let $A \in \mathbb{R}^{2n, 2n}$ be Hamiltonian and have the eigenvalues $\lambda_1, \dots, \lambda_{2n}$ with multiplicities counted. Suppose that there exists an n -dimensional real Lagrangian invariant subspace \mathcal{D} of A corresponding to eigenvalues $\lambda_1, \dots, \lambda_n$ with multiplicities counted. Then*

$$(A - \lambda_1 I) \cdots (A - \lambda_n I) e_1$$

is contained in the Lagrangian A -invariant subspace corresponding to the eigenvalues $\lambda_{n+1}, \dots, \lambda_{2n}$.

(ii) *Let $A \in \mathbb{R}^{2n, 2n}$ be symplectic and have the eigenvalues $\lambda_1, \dots, \lambda_{2n}$ with multiplicities counted. Suppose that there exists an n -dimensional real Lagrangian invariant subspace \mathcal{D} of A corresponding to the eigenvalues $\lambda_1, \dots, \lambda_n$ with multiplicities counted. Then*

$$(A - \lambda_1 I) \cdots (A - \lambda_n I) e_1$$

is contained in the Lagrangian A -invariant subspace corresponding to the eigenvalues $\lambda_{n+1}, \dots, \lambda_{2n}$.

Proof. The proof of (i) and (ii) is immediate from the fact that the invariant subspace corresponding to $\lambda_{n+1}, \dots, \lambda_{2n}$ is the Lagrangian subspace $J\mathcal{D}$. ■

In most applications of the linear regulator problem, one has a Hamiltonian matrix with exactly n eigenvalues in the left half plane and n eigenvalues in the right half plane, and one is interested in computing the *stable* invariant subspace corresponding to the eigenvalues in the left half plane (see, e.g., [12]). But there are also examples in H_∞ -control where a Lagrangian invariant subspace of a Hamiltonian matrix with eigenvalues on the imaginary axis has to be computed; see, e.g., [7]. Such a Hamiltonian matrix has a Lagrangian invariant subspace provided that its purely imaginary eigenvalues occur with even multiplicity (see, e.g., [11]). Proposition 3.1 implies that we can compute a particular Lagrangian invariant subspace of a Hamiltonian matrix as follows:

ALGORITHM 3.2.

Input: A Hamiltonian matrix $A \in \mathbb{R}^{2n, 2n}$ having an n -dimensional Lagrangian invariant subspace \mathcal{D} corresponding to the eigenvalues $\lambda_1, \dots, \lambda_n$, and a tolerance eps .

Output: A real orthogonal symplectic matrix $Q \in \mathbb{R}^{2n, 2n}$ such that the first n columns of Q span the Lagrangian subspace of A corresponding to the other eigenvalues $\lambda_{n+1}, \dots, \lambda_{2n}$ of A .

Set $Q := I$.

Step 1 (Computation of eigenvalues). Compute the eigenvalues of A with the method of Van Loan [23]. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues corresponding to the required Lagrangian subspace.

Step 2 (Computation of the first column of the transformation matrix and reduction). Form

$$(3.3) \quad x = (A - \lambda_1 I) \cdots (A - \lambda_n I) e_1,$$

and let $Q_1 \in \mathbb{R}^{2n, 2n}$ be an orthogonal symplectic matrix such that

$$Q_1^T x = \alpha e_1, \quad \alpha = \|x\|_2.$$

Set

$$(3.4) \quad A := Q_1^T A Q_1, \quad Q := Q Q_1,$$

and reduce A to the condensed form described in [20] leaving the first

column of Q invariant; i.e., compute an orthogonal symplectic matrix $Q_2 \in \mathbb{R}^{2n, 2n}$ with $Q_2 e_1 = e_1$ such that

$$(3.5) \quad Q_2^T A Q_2 \triangleq \begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix}.$$

Set

$$(3.6) \quad A := Q_2^T A Q_2, \quad Q := Q Q_2.$$

Step 3 (Deflation).

FOR $l = 1, 2, \dots$

FOR $i = 1, \dots, n$

IF $|a_{n+i, i}| < \text{eps}$ THEN set $a_{n+i, i} := 0$.

END FOR

FOR $i = 2, \dots, n$

IF $|a_{i, i-1}| < \text{eps}$ THEN set $a_{i, i-1} := 0$.

END FOR

Let $p \geq 0$ be the largest integer in $\{l, \dots, n\}$ such that $a_{p+1, p} = 0$ and $a_{n+k, k} = 0$ for $k = 1, \dots, p$.

Partition A as

$$(3.7) \quad \begin{bmatrix} F_{11} & F_{12} & G_{11} & G_{12} \\ 0 & F_{22} & G_{21} & G_{22} \\ 0 & 0 & -F_{11}^T & 0 \\ 0 & H_{22} & -F_{12}^T & -F_{22}^T \end{bmatrix} \begin{matrix} \} p \\ \} n-p \\ \} p \\ \} n-p \end{matrix}$$

IF $p = n$ THEN

STOP

ELSE

Set $A_{22} := \begin{bmatrix} F_{22} & G_{22} \\ H_{22} & -F_{22}^T \end{bmatrix}$ and

$$(3.8) \quad x_2 := (A_{22} - \lambda_1 I) \cdots (A_{22} - \lambda_n I) e_1,$$

and compute an orthogonal symplectic matrix

$$Q_2 = \begin{bmatrix} U_2 & V_2 \\ -V_2 & U_2 \end{bmatrix} \in \mathbb{R}^{2(n-p), 2(n-p)}$$

such that $Q_2^T x_2 = a_2 e_1$.

$$(3.9) \quad Q_1 := \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & U_2 & 0 & V_2 \\ 0 & 0 & I & 0 \\ 0 & -V_2 & 0 & U_2 \end{bmatrix} \left. \begin{matrix} \\ \\ \\ \end{matrix} \right\} p,$$

$$A := \tilde{Q}_1^T A \tilde{Q}_1, \quad Q := Q \tilde{Q}_1,$$

and reduce A to the condensed form in [20] again, leaving the first column of Q invariant.

END IF

END FOR

END

An analogous algorithm applies to the symplectic case. The analogue for symplectic matrices of the condensed form in (3.5) is the symplectic matrix

$$\begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix},$$

which can be obtained exactly like that in (3.5). The partitioning in (3.7) becomes

$$(3.10) \quad \begin{bmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ 0 & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ 0 & S_{42} & S_{43} & S_{44} \end{bmatrix}$$

with S_{31} strictly upper triangular and S_{11} upper Hessenberg.

In exact arithmetic, the vector x in (3.3) will be contained in the required Lagrangian invariant subspace \mathcal{Q} , and the integer p in step 3 will be equal to the dimension of the smallest isotropic A -invariant subspace that contains x ; consequently, $p \geq 1$. If $p = n$, then the algorithm terminates. Otherwise a

deflation takes place, and the first p columns of Q span the p -dimensional isotropic invariant subspace \mathcal{D}_p that contains x . The vector x_2 in (3.8) is then in $\mathcal{D} \setminus \mathcal{D}_p$, and we can proceed with the deflated matrix.

Steps 2 and 3 of this algorithm use only orthogonal symplectic transformations and thus in exact arithmetic leave the Hamiltonian and symplectic structure invariant. Due to roundoff errors, however, these structures are only retained approximately. It is easy to enforce Hamiltonian structure in order to obtain a nearby Hamiltonian matrix again. In the symplectic case this is not so easy. In fact we do not know how to obtain a close symplectic matrix in an easy way. Difficulties like this have already been observed in other algorithms for symplectic matrices [8].

Even if the eigenvalues in step 1 or the vector x in (3.3) are inaccurate due to roundoff errors, the matrix itself is only transformed with orthogonal symplectic similarity transformations, i.e., if we enforce the structure, in the Hamiltonian case we will obtain the exact similarity transformation of a nearby Hamiltonian matrix.

Several potential difficulties must be addressed in order to develop Algorithm 3.2 into a practical numerical procedure. One such aspect is the fact that the vector x computed by (3.3) will not lie precisely in the desired invariant subspace due to roundoff errors. Of course, this problem is compounded by the inaccuracies in the computed eigenvalues. The components of x in the undesired eigendirections may cause the algorithm to produce elements $a_{j+n,j}$ that are not tiny, and a deflation step will then be performed. Moreover, there is no guarantee that $p > 0$. If too many such deflation steps are required, then the algorithm will not be competitive. The possibility of developing Algorithm 3.2 into a practical numerical procedure is currently under investigation.

4. CONCLUSION

We have shown that the first column of an orthogonal symplectic matrix that transforms a Hamiltonian matrix to Hamiltonian Hessenberg form or a symplectic matrix to symplectic Hessenberg form can be characterized in terms of the solution of a system of quadratic equations. In the case that the resulting Hessenberg-like matrix is unreduced with positive subdiagonal-type elements, the transformation is uniquely determined by its first column. Our characterization provides insight into problems involving these reductions of Hamiltonian and symplectic matrices. For example, the existence of a Hessenberg reduction can be concluded from the solvability of these equations. Moreover, any numerical procedure for such reductions must provide a

solution of these quadratic equations. The characterization therefore also indicates the complexity of an algorithm for the reduction of a general Hamiltonian or symplectic matrix.

These considerations then led us to propose a structure-preserving method for computing the stable deflating subspace of a Hamiltonian or symplectic matrix, which provides an approach to the solution of algebraic Riccati equations.

Future work along these lines will include consideration of the practical implementation of this method as well as the extension of these results to Hamiltonian and symplectic pencils.

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