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# A Numerically Stable, Structure Preserving Method for Computing the Eigenvalues of Real Hamiltonian or Symplectic Pencils

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# A Numerically Stable, Structure Preserving Method for Computing the Eigenvalues of Real Hamiltonian or Symplectic Pencils

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**Abstract**

A new method is presented for the numerical computation of the generalized eigenvalues of real Hamiltonian or symplectic pencils and matrices. The method is strongly backward stable, i.e., it is numerically backward stable and preserves the structure (i.e., Hamiltonian or symplectic). In the case of a Hamiltonian matrix the method is closely related to the square reduced method of Van Loan, but in contrast to that method which may suffer from a loss of accuracy of order $\sqrt{\varepsilon}$, where $\varepsilon$ is the machine precision, the new method computes the eigenvalues to full possible accuracy.

**Keywords.** eigenvalue problem, Hamiltonian pencil (matrix), symplectic pencil (matrix), skew-Hamiltonian matrix
**AMS subject classification.** 65F15

## 1 Introduction

The eigenproblem for Hamiltonian and symplectic matrices has received a lot of attention in the last 25 years, since the landmark papers of Laub [13] and Paige/Van Loan [20]. The reason for this is the importance of this problem in many applications in control theory and signal processing, [17, 12] and also due to the fact that the construction of a completely satisfactory method is still an open problem. Such a method should be numerically backward stable, have a complexity of $O(n^3)$ or less and at the same time preserve the Hamiltonian or symplectic structure. Many attempts have been made to tackle this problem, see [8, 15, 17] and the references therein, but it has been shown in [2] that a modification of standard QR-like methods to solve this problem is in general hopeless, due to the missing reduction to a Hessenberg–like form. For this reason other methods like the multishift-method of [1] were developed that do not follow the direct line of a standard QR-like method. The structure of the multishift method is at first a computation of the eigenvalues followed by a sequence

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of exact-shift steps of a QR method that is based on the non-Hessenberg reduction of Paige and Van Loan [20]. The method is backward stable and structure preserving but it may suffer from loss of convergence, in particular for large problems and furthermore it needs good approximations for the eigenvalues first. These can for example be obtained via the square-reduced method of Van Loan [25]. In the symplectic case a similar method has been proposed by Lin [16] and improved by Patel [21]. Both methods are structure preserving and backward stable for a modified problem which involves the square of the original matrix. But squaring a matrix, computing the eigenvalues of the square, and taking square roots to obtain the eigenvalues of the original matrix can lead to a loss of half of the possible accuracy. This was shown by the worst-case error analysis in [25].

In this paper we will present a new method which does not suffer from this loss of accuracy and it is constructed in such a way that the same method can be used for Hamiltonian matrices, symplectic matrices, Hamiltonian pencils, or symplectic pencils. The method is structure preserving, backward stable, and needs $O(n^3)$ floating point operations. There are three main ingredients for this new method, a new matrix decomposition, which can be viewed as a symplectic URV decomposition, a periodic Schur decomposition for a product of two or four matrices [6, 10, 11] and the generalized Cayley transformation which allows a unified treatment of Hamiltonian and symplectic problems, [14, 18].

The paper is organized as follows: In Section 2 we introduce the notation and review some basic results. In Section 3 we develop the theoretical basis for the new algorithm and in Section 4 we then describe the new procedure. An error analysis is given in Section 5 and numerical examples are presented in Section 6.

## 2 Notation and Preliminaries

In this section we introduce some notation, important definitions and also some preliminary results.

We will be concerned with the computation of eigenvalues of special matrices and matrix pencils. To simplify the notation we use in the following the expression *eigenvalue* for eigenvalues of matrices and also for pairs $(\alpha, \beta) \neq (0,0)$ for which the determinant of a matrix pencil $\alpha E - \beta A$ vanishes. These pairs are not unique, since they can be scaled by a nonzero factor and still the determinant vanishes. So if $\beta \neq 0$ then we identify $(\alpha, \beta)$ with $(\frac{\alpha}{\beta}, 1)$ or $\lambda = \frac{\alpha}{\beta}$. Pairs $(\alpha, 0)$ with $\alpha \neq 0$ are called *infinite eigenvalues.*

We now introduce the classes of matrices and matrix pencils that are discussed in this paper.

**Definition 1** *Let* $J := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, *where* $I_n$ *is the* $n \times n$ *identity matrix.*

*a) A pencil* $\alpha\mathcal{E} - \beta\mathcal{A} \in \mathbf{R}^{2n\times 2n}$ *is called* **Hamiltonian** *iff* $\mathcal{E}J\mathcal{A}^T = -\mathcal{A}J\mathcal{E}^T$. *The set of Hamiltonian pencils in* $\mathbf{R}^{2n\times 2n}$ *is denoted by* $\mathbf{H^P_{2n}}$.
*b) A matrix* $\mathcal{H} \in \mathbf{R}^{2n\times 2n}$ *is called* **Hamiltonian** *iff* $(\mathcal{H}J)^T = \mathcal{H}J$. *The Lie Algebra of Hamiltonian matrices in* $\mathbf{R}^{2n\times 2n}$ *is denoted by* $\mathbf{H_{2n}}$.
*c) A matrix* $\mathcal{H}_s \in \mathbf{R}^{2n\times 2n}$ *is called* **skew-Hamiltonian** *iff* $(\mathcal{H}_sJ)^T = -\mathcal{H}_sJ$. *The set of skew-Hamiltonian matrices in* $\mathbf{R}^{2n\times 2n}$ *is denoted by* $\mathbf{SH_{2n}}$.
*d) A pencil* $\alpha\mathcal{E} - \beta\mathcal{A} \in \mathbf{R}^{2n,2n}$ *is called* **symplectic** *iff* $\mathcal{E}J\mathcal{E}^T = \mathcal{A}J\mathcal{A}^T$. *The set of symplectic pencils in* $\mathbf{R}^{n\times n}$ *is denoted by* $\mathbf{S^P_{2n}}$.

*e) A matrix $\mathcal{S} \in \mathbf{R}^{n\times n}$ is called* **symplectic** *iff $\mathcal{S}J\mathcal{S}^T = J$. The Lie group of symplectic matrices in $\mathbf{R}^{n\times n}$ is denoted by $\mathbf{S_{2n}}$.*
*f) A matrix $\mathcal{U} \in \mathbf{R}^{2n\times 2n}$ is called* **orthogonal symplectic** *iff $\mathcal{U}J\mathcal{U}^T = J$ and $\mathcal{U}\mathcal{U}^T = I_{2n}$. The Lie group of orthogonal symplectic matrices in $\mathbf{R}^{2n\times 2n}$ is denoted by $\mathbf{US_{2n}}$.*

In this paper we will mainly discuss regular Hamiltonian and symplectic pencils, (a pencil $\alpha E - \beta A$ is called *regular* if $\det(\alpha E - \beta A)$ does not vanish identically for all complex pairs $(\alpha, \beta)$.) The main reasons for this are first that we do not know of any application for singular Hamiltonian or symplectic pencils and second that for singular pencils no eigenvalue computation is necessary, since every complex number is an eigenvalue. We will, however, point out in our algorithm when we detect singularity or near singularity of the pencil.

We have the following well-known properties of Hamiltonian and symplectic pencils:

**Proposition 1**
*a) Let $\alpha\mathcal{E} - \beta\mathcal{A}$ be a real Hamiltonian pencil. If $\mu = \frac{\alpha}{\beta}$ is a finite eigenvalue of $\alpha\mathcal{E} - \beta\mathcal{A}$, then also $-\bar{\mu}$, $\bar{\mu}$, $-\mu$ are eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$.*
*b) Let $\alpha\mathcal{E} - \beta\mathcal{A}$ be a real symplectic pencil. If $\mu = \frac{\alpha}{\beta}$ is an eigenvalue of $\alpha\mathcal{E} - \beta\mathcal{A}$, then also $1/\bar{\mu}$, $\bar{\mu}$, $1/\mu$ are eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$. This includes the eigenvalue $0$ corresponding to $(\alpha, \beta) = (0, 1)$ with infinite eigenvalue $(\alpha, \beta) = (1, 0)$ as counterpart.*
*c) Any matrix $\mathcal{H} \in \mathcal{H}_{2n}$ can be written as $\mathcal{H} = \begin{bmatrix} F & G \\ H & -F^T \end{bmatrix}$, where $F$, $G$, $H \in \mathbf{R}^{n\times n}$ and $G = G^T$, $H = H^T$.*
*d) Any matrix $\mathcal{U} \in \mathbf{US_{2n}}$ can be written as $\mathcal{U} = \begin{bmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{bmatrix}$, where $U_1, U_2 \in \mathbf{R}^{n\times n}$.*

*Proof.* See, e.g., [15, 17]. □

There is a well-known relationship between Hamiltonian and symplectic pencils, which is given via the generalized Cayley transformation, e.g., [14, 18] and there is also an interesting relationship between Hamiltonian and skew-Hamiltonian matrices, which, however, does not extend to pencils.

**Lemma 2**
*a) Let $\alpha\mathcal{E}_s - \beta\mathcal{A}_s$ be a real symplectic pencil and let $\lambda_1 = 1$ or $\lambda_1 = -1$.*
*Then*

$$\alpha\mathcal{E}_H - \beta\mathcal{A}_H := \alpha(\mathcal{E}_s - \lambda_1\mathcal{A}_s) - \beta(\lambda_1\mathcal{E}_s + \mathcal{A}_s) \tag{1}$$

*is a real Hamiltonian pencil.*
*b) Let $\alpha\mathcal{E}_H - \beta\mathcal{A}_H$ be a real Hamiltonian pencil and let $\lambda_1 = 1$ or $\lambda_1 = -1$. Then*

$$\alpha\mathcal{E}_s - \beta\mathcal{A}_s = \alpha(\lambda_1\mathcal{A}_H + \mathcal{E}_H) - \beta(\mathcal{A}_H - \lambda_1\mathcal{E}_H) \tag{2}$$

*is a real symplectic pencil.*
*c) Let $\mathcal{H}$ be a Hamiltonian matrix, then $\mathcal{H}^2$ is skew Hamiltonian.*

*Proof.* For a) and b) see [14, 18], for c) see [25]. □

Further properties of symplectic and Hamiltonian pencils are discussed in [14, 15, 17, 18].

**Remark 1** For Hamiltonian pencils $\alpha\mathcal{E} - \beta\mathcal{A}$ with $\mathcal{E}$ invertible, Part c) of Lemma 2 suggests that the pencil

$$\alpha\mathcal{E}J\mathcal{E}^T - \beta\mathcal{A}J^T\mathcal{A}^T \tag{3}$$

might be a skew-Hamiltonian pencil, i.e.,

$$\mathcal{E}J\mathcal{E}^T J\mathcal{A}J\mathcal{A}^T = \mathcal{A}J\mathcal{A}^T J\mathcal{E}J\mathcal{E}^T. \tag{4}$$

However, in general this is not the case, since to show this we would also need that $\mathcal{E}^T J\mathcal{A} = -\mathcal{A}^T J\mathcal{E}$ for the Hamiltonian pencil. But this holds only in some special cases. If, for example, one of the matrices $\mathcal{E}$ or $\mathcal{A}$ is symplectic or if $\mathcal{E}^{-1}$ and $\mathcal{A}$ commute, then (3) is a skew-Hamiltonian pencil. In general this is not true as the following example shows.

**Example 1** *Let*

$$\mathcal{E} = \begin{bmatrix} 2 & 0 & 2 & 1 \\ 2 & 4 & 1 & 4 \\ -1 & -1 & 2 & 2 \\ -1 & -2 & 0 & 4 \end{bmatrix}, \qquad \mathcal{A} = \begin{bmatrix} 0 & 0 & 2 & 1 \\ -2 & -2 & 1 & 4 \\ 1 & 1 & 0 & 2 \\ 1 & 2 & 0 & 2 \end{bmatrix}.$$

*The pencil $\alpha\mathcal{E} - \beta\mathcal{A}$ is Hamiltonian according to Definition 1 as can easily be checked by computing $\mathcal{A}J\mathcal{E}^T + \mathcal{E}J\mathcal{A}^T$, but*

$$\mathcal{A}^T J\mathcal{E} + \mathcal{E}^T J\mathcal{A} = \begin{bmatrix} 0 & 4 & 0 & 0 \\ -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 12 \\ 0 & 0 & -12 & 0 \end{bmatrix}$$

*and*

$$\mathcal{E}J\mathcal{E}^T J\mathcal{A}J\mathcal{A}^T - \mathcal{A}J\mathcal{A}^T J\mathcal{E}J\mathcal{E}^T = \begin{bmatrix} 0 & -48 & -32 & -32 \\ 48 & -96 & -8 & 32 \\ -32 & -8 & -32 & -16 \\ -32 & 32 & -16 & 0 \end{bmatrix}.$$

On the other hand, as we will show below, this does not harm the spectral properties, i.e., we can still use (3) to compute the eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$.

# 3 Theoretical Background

When one does eigenvalue computations one is usually restricted to similarity transformations for matrices and equivalence transformations for pencils, since only these preserve all the spectral properties.

The basis for our new algorithm, however, is a non-equivalence transformation for the original Hamiltonian pencil, which leads to an equivalence transformation for the pencil (3). From the eigenvalues of (3) we can then easily compute the eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$.

**Lemma 3**
*a) Let $\alpha\mathcal{E} - \beta\mathcal{A}$ be a regular real Hamiltonian pencil. The pair $(\mu, \nu)$ is an eigenvalue of the pencil $\alpha\mathcal{E}J\mathcal{E}^T - \beta\mathcal{A}J^T\mathcal{A}^T$ if and only if the pairs $(\sqrt{\mu}, \sqrt{\nu})$, $(-\sqrt{\mu}, \sqrt{\nu})$ are eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$.*
*b) If $\lambda \neq 0$ is a simple eigenvalue of a Hamiltonian matrix $\mathcal{H}$ then $\lambda^2$ is a nondefective eigenvalue of $\mathcal{H}^2$ of multiplicity 2.*

*Proof.* The eigenvalues of $\alpha\mathcal{E}-\beta\mathcal{A}$ are the pairs $(\mu,\nu)\neq(0,0)$ for which $\det(\mu\mathcal{E}-\nu\mathcal{A})=0$. Now $\det(\mu\mathcal{E}-\nu\mathcal{A})=0$ if and only if

$$\begin{aligned}\det[(\mu\mathcal{E}-\nu\mathcal{A})J(\mu\mathcal{E}-\nu\mathcal{A})^T] &= \det(\mu^2\mathcal{E}J\mathcal{E}^T-\mu\nu(\mathcal{E}J\mathcal{A}^T+\mathcal{A}J\mathcal{E}^T)-\nu^2\mathcal{A}J^T\mathcal{A}^T)\\ &= \det(\mu^2\mathcal{E}J\mathcal{E}^T-\nu^2\mathcal{A}J^T\mathcal{A}^T)=0,\end{aligned}$$

and hence a) follows.

For b) observe that if $\lambda\neq 0$ is a simple finite eigenvalue of $\mathcal{H}$, then also $-\lambda$ is a simple eigenvalue. Let $x_1,x_2$ be the corresponding right eigenvectors, which are clearly independent if $\lambda\neq 0$. Any linear combination of $x_1$ and $x_2$ then is a right eigenvector of $\mathcal{H}^2$, and hence the dimension of the eigenspace is two and $\lambda^2$ is a nondefective double eigenvalue. □

**Remark 2** From the proof of Lemma 3 b), we see that the eigenvalue condition number $1/s(\lambda)$ is not uniquely defined for the eigenvalues $\lambda^2$ of $\mathcal{H}^2$. Since $s(\lambda)=y^Hx$, where $y$ and $x$ are the left and right eigenvectors of $H$ corresponding to $\lambda$, $1/s(\lambda)$ can also be considered as a condition number of $\lambda^2$ with respect to $\mathcal{H}^2$ is given by. But since any linear combination of $x_1$ and $x_2$ from the proof of Part b) defines a right eigenvector of $\mathcal{H}^2$ corresponding to $\lambda^2$ and any linear combination of the left eigenvectors $y_1$ and $y_2$ of $\mathcal{H}$ corresponding to $\lambda$ and $-\lambda$, respectively, defines a left eigenvector of $\mathcal{H}^2$ corresponding to $\lambda^2$, many other values for $s(\lambda^2)$ with respect to $\mathcal{H}^2$ are possible.

Lemma 3 indicates a way to compute the eigenvalues of a Hamiltonian pencil via the square roots of the eigenvalues of another pencil. This is the direct generalization of the square reduced method of Van Loan [25] to Hamiltonian pencils. If we apply this trick explicitly or implicitly as in the square reduced method, we will suffer from the same $\sqrt{\varepsilon}$ perturbation in the computed eigenvalues as in Van Loan's method.

But in this situation we can apply a trick which is based on a non-equivalence transformation applied to the Hamiltonian pencil. This transformation can be viewed as a symplectic version of the URV-decomposition. URV-decompositions of a matrix into a product of two unitary matrices $U$, $V$ and an upper triangular matrix $R$, were first introduced by Stewart in order to achieve a compromise between accuracy and computational cost between the QR decomposition and the singular value decomposition for rank and nullspace computations, see [23, 22].

In general such decompositions are not useful for the computation of eigenvalues, but as we will see, in the case of Hamiltonian and symplectic pencils or matrices the situation is different.

**Lemma 4** *Let $\alpha E-\beta A$ be a real $2n\times 2n$ pencil. Then there exist orthogonal transformation matrices $Q_3\in\mathbf{R}^{2n\times 2n}$ and $Q_1,Q_2\in\mathbf{US_{2n}}$, (which can be obtained via a finite elimination procedure), such that*

$$Q_3^TEQ_1 = \begin{bmatrix} E_{11} & E_{12}\\ 0 & E_{22}\end{bmatrix}, \tag{5}$$

$$Q_3^TAQ_2 = \begin{bmatrix} A_{11} & A_{12}\\ 0 & A_{22}\end{bmatrix}, \tag{6}$$

*where $E_{ij},A_{ij}\in\mathbf{R}^{n\times n}$, $E_{11}$, $A_{11}$, $E_{22}^T$ are upper triangular, and $A_{22}^T$ is upper Hessenberg.*

*Proof.* The proof is given in a constructive way by Algorithm 3 in the next section. □

Lemma 4 describes a finite step non-equivalence transformation to a condensed form. This form is a mixture between the Hessenberg and the triangular form for real $2n \times 2n$ pencils. The second result that we need is that the Hessenberg matrix $A_{22}$ in Lemma 4 can also be transformed to quasi-upper triangular form with the same type of transformations.

**Theorem 5** *Let $\alpha E - \beta A$ be a real $2n \times 2n$ pencil. Then there exist orthogonal transformation matrices $Q_3 \in \mathbf{R}^{2n\times 2n}$ and $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that*

$$Q_3^T E Q_1 = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix}, \; Q_3^T A Q_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}, \tag{7}$$

*where $E_{ij}, A_{ij} \in \mathbf{R}^{n\times n}$, $E_{11}$, $A_{11}$, $E_{22}^T$ are upper triangular and $A_{22}^T$ is quasi-upper triangular, i.e., block upper triangular with diagonal blocks of size $1 \times 1$ and $2 \times 2$.*

*Proof.* By Lemma 4 we may assume, w.l.o.g., that the blocks $E_{11}$, $A_{11}$, $E_{22}^T$ are upper triangular and $A_{22}^T$ is upper Hessenberg. We then apply the generalized real Schur decomposition, [[9], p.396] to the pencil $\alpha E_{11}E_{22}^T - \beta A_{11}A_{22}^T$. It follows that there exist real orthogonal matrices $U, V \in \mathbf{R}^{n\times n}$ such that $U^T E_{11} E_{22}^T V$ is upper triangular and $U^T A_{11} A_{22}^T V$ is quasi-upper triangular. Let $U_1, U_2 \in \mathbf{R}^{n\times n}$ be orthogonal matrices such that $U_1^T E_{22}^T V$ and $U^T A_{11} U_2$ are upper triangular (these always exist from the QR factorization). Then it follows that $U^T E_{11} U_1$ is upper triangular and $U_2^T A_{22}^T V$ is quasi-upper triangular. Thus,

$$\alpha \begin{bmatrix} U^T & 0 \\ 0 & V^T \end{bmatrix} E \begin{bmatrix} U_1 & 0 \\ 0 & U_1 \end{bmatrix} - \beta \begin{bmatrix} U^T & 0 \\ 0 & V^T \end{bmatrix} A \begin{bmatrix} U_2 & 0 \\ 0 & U_2 \end{bmatrix}$$

yields the required decomposition. □

For real $2n \times 2n$ matrices we have the following obvious corollary:

**Corollary 6** *Let $A \in \mathbf{R}^{2n\times 2n}$. Then there exist matrices $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that*

$$Q_1^T A Q_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}, \tag{8}$$

*where $A_{ij} \in \mathbf{R}^{n\times n}$, $A_{11}$ is upper triangular and $A_{22}^T$ is quasi-upper triangular.*

*Proof.* The proof follows directly from Theorem 5 by inverting $Q_3^T A Q_1$. □

At first sight it is not clear how the above non-equivalence transformation can be used for eigenvalue computation, but when we apply the transformation to a Hamiltonian pencil $\alpha\mathcal{E} - \beta\mathcal{A}$ and then consider the impact of this transformation on the pencil

$$\alpha\mathcal{E}J\mathcal{E}^T - \beta\mathcal{A}J^T\mathcal{A}^T \tag{9}$$

then we obtain the following result.

**Theorem 7** *Let $\alpha\mathcal{E} - \beta\mathcal{A}$ be a real Hamiltonian pencil. Then there exists an orthogonal matrix $Q_3$ such that*

$$Q_3^T \mathcal{E} J \mathcal{E}^T Q_3 J = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix} \begin{bmatrix} -E_{22}^T & E_{12}^T \\ 0 & -E_{11}^T \end{bmatrix}, \tag{10}$$

*and*

$$Q_3^T \mathcal{A} J^T \mathcal{A}^T Q_3 J = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} A_{22}^T & -A_{12}^T \\ 0 & A_{11}^T \end{bmatrix}, \tag{11}$$

*where $E_{ij}, A_{ij} \in \mathbf{R}^{n\times n}$, $E_{11}$, $A_{11}$, $E_{22}^T$ are upper triangular and $A_{22}^T$ is quasi-upper triangular.*

*Proof.* Applying the transformation from Theorem 5 we obtain

$$\begin{aligned} Q_3^T \mathcal{E} J \mathcal{E}^T Q_3 J &= Q_3^T \mathcal{E} Q_1 J Q_1^T \mathcal{E}^T Q_3 J \\ &= \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix} J \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix}^T J \\ &= \begin{bmatrix} -E_{11}E_{22}^T & E_{11}E_{12}^T - E_{12}E_{11}^T \\ 0 & -(E_{11}E_{22}^T)^T \end{bmatrix} \end{aligned} \tag{12}$$

$$\begin{aligned} Q_3^T \mathcal{A} J^T \mathcal{A}^T Q_3 J &= Q_3^T \mathcal{A} Q_2 J^T Q_2^T \mathcal{A}^T Q_3 J \\ &= \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} J^T \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}^T J \\ &= \begin{bmatrix} A_{11}A_{22}^T & -A_{11}A_{12}^T + A_{12}A_{11}^T \\ 0 & (A_{11}A_{22}^T)^T \end{bmatrix}. \end{aligned} \tag{13}$$

□

An obvious corollary is obtained for Hamiltonian matrices.

**Corollary 8** *Let $\mathcal{H} \in \mathcal{H}_{2n}$ then there exist $Q_1, Q_2 \in \mathbf{US_{2n}}$ such that*

$$Q_1^T \mathcal{H}^2 Q_1 = \begin{bmatrix} -H_{11}H_{22}^T & H_{11}H_{12}^T - H_{12}H_{11}^T \\ 0 & -H_{22}H_{11}^T \end{bmatrix}, \tag{14}$$

$$Q_2^T \mathcal{H}^2 Q_2 = \begin{bmatrix} -H_{22}^T H_{11} & H_{12}^T H_{22} - H_{22}^T H_{12} \\ 0 & -H_{11}^T H_{22} \end{bmatrix}, \tag{15}$$

*with $H_{ij} \in \mathbf{R}^{n\times n}$, $H_{11}$ is upper triangular and $H_{22}^T$ is quasi-upper triangular.*

*Proof.* Using the Hamiltonian structure and $Q_1, Q_2$ from Corollary 6 we obtain that

$$Q_1^T \mathcal{H}^2 Q_1 = Q_1^T \mathcal{H} Q_2 Q_2^T J \mathcal{H}^T J Q_1 = (Q_1^T \mathcal{H} Q_2) J (Q_1^T \mathcal{H} Q_2)^T J,$$

which has the required form. The proof for (15) follows analogously. □

From these two results we see that in order to compute the eigenvalues of $\alpha\mathcal{E} - \beta\mathcal{A}$ it suffices to compute the eigenvalues of the pencil

$$\alpha E_{11} E_{22}^T + \beta A_{11} A_{22}^T \tag{16}$$

as it arises from (10) and (11), and to compute the eigenvalues of a Hamiltonian matrix it suffices to compute the eigenvalues of

$$-H_{11}H_{22}^T \quad \text{or} \quad -H_{22}^T H_{11} \tag{17}$$

as in (14), (15).

Now fortunately we can compute the eigenvalues of (16), (17) from the condensed form of Lemma 3 without forming the products. To do this we can directly employ the periodic Schur decomposition for products of matrices or pencils of products of matrices [6, 10, 11] without forming the products. The periodic QR algorithm applied to (17) yields real orthogonal transformation matrices $U, V \in \mathbf{R}^{n\times n}$ such that

$$\hat{H} := U^T H_{11} V V^T H_{22}^T U, \qquad \hat{H}_{22}^T := (U^T H_{22} V)^T \tag{18}$$

are quasi-upper triangular, while

$$\hat{H}_{11} := U^T H_{11} V \tag{19}$$

is upper triangular. Analogously the periodic QZ-algorithm applied to (16) yields real orthogonal transformation matrices $U, V, Y, Z \in \mathbf{R}^{n\times n}$ such that

$$\begin{array}{rcl} \hat{E} & := & U^T E_{11} V V^T E_{22}^T Z, \qquad \hat{E}_{11} := U^T E_{11} V, \\ \hat{E}_{22}^T & := & (Z^T E_{22} V)^T, \qquad \hat{A}_{11} := U^T A_{11} Y \end{array} \tag{20}$$

are upper triangular and

$$\hat{A} := U^T A_{11} Y Y^T A_{22}^T Z, \qquad \hat{A}_{22}^T := (Z^T A_{22} Y)^T \tag{21}$$

are quasi-upper triangular. After these forms have been computed, we can compute the eigenvalues of $\hat{H}$ or $\alpha\hat{E} - \beta\hat{A}$, respectively by solving $1\times 1$ or $2\times 2$ eigenvalue problems. We present here the formulas for the pencil situation, the matrix case is obtained by setting $\hat{E} = I_n$. Let

$$\begin{array}{rcl} \hat{E}_{11} & := & U^T E_{11} V =: [e_{ij}], \\ \hat{E}_{22} & := & Z^T E_{22} V =: [f_{ij}], \\ \hat{A}_{11} & := & U^T A_{11} Y =: [a_{ij}], \\ \hat{A}_{22} & := & Z^T A_{22} Y =: [b_{ij}]. \end{array} \tag{22}$$

In the case of a $1\times 1$ diagonal block in $\hat{A}_{22}$ the corresponding eigenvalue is a solution of the equation

$$\mu(e_{ii} f_{ii}) + \nu(a_{ii} b_{ii}) = 0, \tag{23}$$

i.e., $(\mu, \nu) = (-\frac{a_{ii}b_{ii}}{e_{ii}f_{ii}}, 1)$ if $e_{ii}f_{ii} \neq 0$ or $(\mu, \nu) = (1, 0) \sim \infty$ if $e_{ii}f_{ii} = 0$ and $a_{ii}b_{ii} \neq 0$. If both products are 0 then the pencil is singular, and thus clearly if both products are close to 0, then the pencil is near to a singular pencil, see [24]. The eigenvalues of the original Hamiltonian pencil are then obtained via Lemma 3.

In the case of an unreduced $2\times 2$ diagonal block in $\hat{A}_{22}$ the corresponding eigenvalue is an eigenvalue of the pencil

$$\mu \begin{bmatrix} e_{ii} & e_{i,i+1} \\ 0 & e_{i+1,i+1} \end{bmatrix} \begin{bmatrix} f_{ii} & f_{i,i+1} \\ 0 & f_{i+1,i+1} \end{bmatrix} + \nu \begin{bmatrix} a_{ii} & a_{i,i+1} \\ 0 & a_{i+1,i+1} \end{bmatrix} \begin{bmatrix} b_{ii} & b_{i,i+1} \\ b_{i+1,i} & b_{i+1,i+1} \end{bmatrix}, \tag{24}$$

which has the characteristic polynomial

$$\mu^2 a + \mu\nu b + \nu^2 c \tag{25}$$

where the coefficients are given by

$$\begin{aligned}
a &= e_{ii}e_{i+1,i+1}f_{ii}f_{i+1,i+1}, \\
b &= e_{ii}f_{ii}a_{i+1,i+1}b_{i+1,i+1} + (a_{ii}b_{ii} + a_{i,i+1}b_{i+1,i})e_{i+1,i+1}f_{i+1,i+1} \\
& \quad -a_{i+1,i+1}b_{i+1,i}(e_{ii}f_{i,i+1} + e_{i,i+1}f_{i+1,i+1}), \\
c &= a_{ii}a_{i+1,i+1}(b_{ii}b_{i+1,i+1} - b_{i+1,i}b_{i,i+1}).
\end{aligned}$$

We obtain that the pencil is singular if $a = b = c = 0$ and it is near to a singular pencil if all three coefficients are close to 0. If this is not the case, then we have the following cases:

There exists one eigenvalue infinity if $a = 0$ and $b \neq 0$ and two infinite eigenvalues if $a = b = 0$ and $c \neq 0$. If $a = 0$ and $b \neq 0$ then the other eigenvalue is $(\mu, \nu) = (\frac{c}{b}, 1)$. If $a \neq 0$ then the eigenvalues are both finite, of the form $(\mu, \nu) = (\lambda_i, 1)$, where $\lambda_i$, $i = 1, 2$, are the solutions of the quadratic equation

$$\lambda^2 + \lambda\frac{b}{a} + \frac{c}{a} = 0.$$

The eigenvalues of the original Hamiltonian pencil are again obtained via Lemma 3.

In this section we have described a new method to compute the eigenvalues of Hamiltonian pencils. We can apply the same idea to symplectic pencils by using the generalized Cayley transformation of Lemma 2 b) to transform the symplectic pencil to a Hamiltonian pencil, applying the described procedure and computing the eigenvalues via the inverse Cayley transformation applied to the eigenvalues.

If $(\alpha, \beta)$ is an eigenvalue of the Hamiltonian pencil obtained via the Cayley transformation with shiftpoint $\lambda_1$, then $(\lambda_1\beta+\alpha, \beta-\lambda_1\alpha)$ is the associated eigenvalue of the original symplectic pencil.

**Remark 3** The method described above can in principle also be applied to a pencil $\alpha E - \beta A$ where $E, A \in \mathbf{R}^{2n\times 2n}$ are skew-symmetric since every skew-symmetric matrix $B \in \mathbf{R}^{2n\times 2n}$ can be factored as $B = CJC^T$.

**Remark 4** Note that the described procedure cannot be applied to complex symplectic or Hamiltonian pencils. The reason for this is that the reduction to condensed form via unitary symplectic matrices cannot be carried out in the same way, since with unitary symplectic matrices less eliminations are possible. The same problem already occurs in the square reduced method of Van Loan [25].

**Remark 5** If we apply Lemma 4 to a symplectic matrix $S$, i.e., we set $E = I_{2n}$ and choose $Q_1 = Q_3$, then

$$Q_1^T S Q_2 = \begin{bmatrix} S_1 & S_2 \\ 0 & S_1^{-T} \end{bmatrix} \tag{26}$$

where $S_1$ is an upper triangular matrix and $S_1S_2^T - S_2S_1^T = 0$, i.e., $Q_1^TSQ_2$ is *symplectic triangular* [17]. In addition, $Q_2 = I_{2n}$ and (26) is equivalent to the symplectic QR decomposition of a symplectic matrix (see [7]).

## 4 The Numerical Algorithm

We have already described the main features of the new algorithm in Section 3.

**Algorithm 1** *A structure preserving method for the computation of the eigenvalues of Hamiltonian and symplectic pencils.*
**Input:** Hamiltonian pencil $\alpha\mathcal{E}_H - \beta\mathcal{A}_H$ or symplectic pencil $\alpha\mathcal{E}_s - \beta\mathcal{A}_s$.
**Output:** Eigenvalues of the pencil.
**Step 0:** If the pencil is symplectic, choose $\lambda_1 \in \{1, -1\}$ and form

$$\alpha\mathcal{E}_H - \beta\mathcal{A}_H := \alpha(\mathcal{E}_s - \lambda_1\mathcal{A}_s) - \beta(\lambda_1\mathcal{E}_s + \mathcal{A}_s).$$

**Step 1:** Determine orthogonal transformation matrices $Q_3 \in \mathbf{R}^{2n\times 2n}$ and $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that

$$Q_3^T\mathcal{E}_H Q_1 = \begin{bmatrix} E_{11} & E_{12} \\ 0 & E_{22} \end{bmatrix}, \qquad Q_3^T\mathcal{A}_H Q_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix},$$

where $E_{ij}, A_{ij} \in \mathbf{R}^{n\times n}$, $E_{11}$, $A_{11}$, $E_{22}^T$ are upper triangular and $A_{22}^T$ is upper Hessenberg (see Algorithm 3).
**Step 2:** Apply the periodic QZ algorithm of [11] to the product pencil

$$\alpha E_{11}E_{22}^T + \beta A_{11}A_{22}^T, \tag{27}$$

i.e., compute orthogonal transformation matrices $U_1, U_2, U_3, U_4 \in \mathbf{R}^{n\times n}$ such that

$$U_1^T E_{11} U_2, \quad (U_3^T E_{22} U_2)^T, \quad U_1^T A_{11} U_4 \tag{28}$$

are upper triangular and

$$(U_3^T A_{22} U_4)^T \tag{29}$$

is quasi-upper triangular.
**Step 3:** Solve the $1\times 1$ or $2\times 2$ eigenvalue problems arising from explicitly multiplying out the diagonal blocks in (27), i.e., determine pairs $(\mu_i, \nu_i)$ for $i = 1, \ldots, n$ via (24) or (25), respectively.
**Step 4:** Compute the finite eigenvalues $(\alpha_i, \beta_i)$ of $\alpha\mathcal{E} - \beta\mathcal{A}$ as

$$\left.\begin{array}{rcl} (\alpha_i, \beta_i) & = & (\sqrt{\mu_i}, \sqrt{\nu_i}), \\ (\alpha_{n+i}, \beta_{n+i}) & = & (-\sqrt{\mu_i}, \sqrt{\nu_i}), \end{array}\right\} \quad i = 1, \ldots, n. \tag{30}$$

**Step 5:** If the original pencil was symplectic, then compute the eigenvalues of $\alpha\mathcal{E}_s - \beta\mathcal{A}_s$ as

$$(\alpha_i^s, \beta_i^s) = (\lambda_1\beta_i + \alpha_i, \beta_i - \lambda_1\alpha_i), \quad i = 1, \ldots, 2n. \tag{31}$$

**End**

The main computational work lies in Steps 1. and 2. of this procedure. While Step 2. is well analyzed, and different procedures for this problem have been described [6, 11], Step 1 is new and we describe it in more detail below.

If we want to apply Algorithm 1 to a Hamiltonian matrix it simplifies significantly. Note that for symplectic matrices we still need to use the pencil formulation, since the associated Hamiltonian problem arising from the Cayley transformation is in general a Hamiltonian pencil.

**Algorithm 2** *A structure preserving method for the computation of the eigenvalues of a Hamiltonian matrix.*

**Input:** Hamiltonian matrix $\mathcal{H}$.

**Output:** The eigenvalues $\{\gamma_1, \ldots, \gamma_{2n}\}$ of $\mathcal{H}$.

**Step 1:** Determine orthogonal transformation matrices $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that

$$Q_1^T \mathcal{H} Q_2 = \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix}, \tag{32}$$

where $H_{ij} \in \mathbf{R}^{n\times n}$, $H_{11}$ is upper triangular, and $H_{22}^T$ is upper Hessenberg.

**Step 2:** Apply the periodic QR algorithm of [10] to the product matrix

$$-H_{22}^T H_{11}, \tag{33}$$

i.e., compute orthogonal transformation matrices $U_1, U_2 \in \mathbf{R}^{n\times n}$ such that

$$U_1^T H_{11} U_2, \tag{34}$$

is upper triangular and

$$(U_1^T H_{22} U_2)^T \tag{35}$$

is quasi-upper triangular.

**Step 3:** Solve the $1\times 1$ or $2\times 2$ eigenvalue problems arising from explicitly multiplying out the diagonal blocks in (34), (35), i.e., determine eigenvalues $\lambda_i$, $i = 1, \ldots, n$, via the solution of the $1\times 1$ or $2\times 2$ eigenvalue problems arising in the block diagonal of this product.

**Step 4:** Compute the eigenvalues of $\mathcal{H}$ by $\quad \gamma_i = \sqrt{\lambda_i}, \quad \gamma_{n+i} = -\sqrt{\lambda_i}, \qquad i = 1, \ldots, n.$

**End**

We now describe the reduction to the condensed form (5), (6). For this reduction we need five basic transformations. These are transformations with Givens rotations and Householder reflections from the left and transformations with three types of orthogonal symplectic matrices from the right. Standard Givens rotations in $\mathbf{R}^{2n\times 2n}$ operating in rows $i, j \in \{1, \ldots, 2n\}$ are of the form

$$J(i,j,\theta) := \begin{bmatrix} I_{i-1} & & & & \\ & \cos(\theta) & & \sin(\theta) & \\ & & I_{j-i-1} & & \\ & -\sin(\theta) & & \cos(\theta) & \\ & & & & I_{2n-j} \end{bmatrix}, \tag{36}$$

while symplectic Givens rotations take the same form but operate in rows $i, n+i$, $i \in \{1, \ldots, n\}$, i.e.,

$$J_s(i,\theta) := J(i, n+i, \theta). \tag{37}$$

The third type of transformations consists of the direct sum of two $n\times n$ Givens rotations. Such matrices operate in rows $i, j, n+i, n+j$, where $i, j \in \{1, \ldots, n\}$ and have the form

$$G_s(i,j,\theta) := \begin{bmatrix} J(i,j,\theta) & 0 \\ 0 & J(i,j,\theta) \end{bmatrix}. \tag{38}$$

Besides the transformations that carry out rotations, we need two types of Householder reflection matrices. A standard Householder reflection in $\mathbf{R}^{n\times n}$ is given by

$$P(k,v) = I_n - 2\frac{vv^T}{v^Tv} \tag{39}$$

where $v_i = 0$ for $i = 1,\ldots,k-1$. A symplectic Householder matrix is defined in [20] as the direct sum of two Householder reflections in $\mathbf{R}^{n\times n}$, i.e.,

$$P_s(k,v) = \begin{bmatrix} P(k,v) & 0 \\ 0 & P(k,v) \end{bmatrix}. \tag{40}$$

Numerical procedures that implement these transformations and their numerical properties are well studied and need not be repeated here, [20, 9, 17]. The condensed form of Lemma 4 is obtained via a sequence of transformations and described in the following Algorithm.

**Algorithm 3** *Reduction of a general real $2n\times 2n$ pencil to the condensed form of Lemma 4.*

**Input:** Real $2n\times 2n$ pencil $\alpha E - \beta A = \alpha \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} - \beta \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$.

**Output:** Orthogonal matrices $Q_3 \in \mathbf{R}^{2n\times 2n}$ and $Q_1, Q_2 \in \mathbf{US_{2n}}$, and transformed pencil

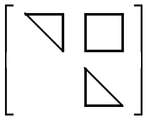
$$\alpha\hat{E} - \beta\hat{A} \;:=\; \alpha Q_3^T E Q_1 - \beta Q_3^T A Q_2 = \alpha \begin{bmatrix} \hat{E}_{11} & \hat{E}_{12} \\ 0 & \hat{E}_{22} \end{bmatrix} - \beta \begin{bmatrix} \hat{A}_{11} & \hat{A}_{12} \\ 0 & \hat{A}_{22} \end{bmatrix},$$

where $\hat{E}_{ij}, \hat{A}_{ij} \in \mathbf{R}^{n\times n}$, $\hat{E}_{11}$, $\hat{A}_{11}$, $\hat{E}_{22}^T$ are upper triangular and $\hat{A}_{22}^T$ is upper Hessenberg.

**Step 1:**

Compute a QR factorization $\begin{bmatrix} E_{11} \\ E_{21} \end{bmatrix} = Q_0 \begin{bmatrix} \hat{E}_{11} \\ 0 \end{bmatrix}$ where $\hat{E}_{11} \in \mathbf{R}^{n\times n}$ is upper triangular and $Q_0 \in \mathbf{U_{2n}}$ and set $\hat{E} \;:=\; Q_0^T E =: \begin{bmatrix} \hat{E}_{11} & \hat{E}_{12} \\ 0 & \hat{E}_{22} \end{bmatrix}$.

Compute a QL factorization $\hat{E}_{22} = \tilde{Q}L$ and set $\tilde{Q}_0 \;:=\; \begin{bmatrix} I_n & 0 \\ 0 & \tilde{Q} \end{bmatrix}$,

$\hat{E} \;:=\; \tilde{Q}_0^T \hat{E} \;=\; \begin{bmatrix} \hat{E}_{11} & \hat{E}_{12} \\ 0 & \hat{E}_{22} \end{bmatrix} \;=$ ,

$\hat{A} \;:=\; \tilde{Q}_0^T Q_0^T A \;=:\; \begin{bmatrix} \hat{A}_{11} & \hat{A}_{12} \\ \hat{A}_{21} & \hat{A}_{22} \end{bmatrix}$,

$Q_3 \;:=\; Q_0\tilde{Q}_0, \quad Q_1 \;:=\; I_{2n}, \quad Q_2 \;:=\; I_{2n}.$

**Step 2:**

For $k = 1,\ldots,n-1$
% *Annihilate $\hat{A}_{n+k:2n,k}$.*
For $j = k,\ldots,n-1$
Use $J(n+j, n+j+1, \theta^{k,j,1})$ to eliminate $\hat{a}_{n+j,k}$ from the left. Set
$\hat{E} \;:=\; J(n+j, n+j+1, \theta^{k,j,1})^T \hat{E}$,
$\hat{A} \;:=\; J(n+j, n+j+1, \theta^{k,j,1})^T \hat{A}$,
$Q_3 \;:=\; Q_3 J(n+j, n+j+1, \theta^{k,j,1})$

Use $G_s(j, j+1, \theta^{k,j,2})$ to eliminate $\hat{e}_{n+j,n+j+1}$ from the right. Set
$\hat{E} := \hat{E} G_s(j, j+1, \theta^{k,j,2})$,
$Q_1 := Q_1 G_s(j, j+1, \theta^{k,j,2})$,
Use $J(j, j+1, \theta^{k,j,3})$ to eliminate $\hat{e}_{j+1,j}$ from the left. Set
$\hat{E} := J(j, j+1, \theta^{k,j,3})^T \hat{E}$,
$\hat{A} := J(j, j+1, \theta^{k,j,3})^T \hat{A}$,
$Q_3 := Q_3 J(j, j+1, \theta^{k,j,3})$.
Endfor $j$
Use $J_s(n, \theta^{k,n,1})$ to eliminate $\hat{a}_{2n,k}$ from the left. Set
$\hat{E} := J_s(n, \theta^{k,n,1})^T \hat{E}$,
$\hat{A} := J_s(n, \theta^{k,n,1})^T \hat{A}$,
$Q_3 := Q_3 J_s(n, \theta^{k,n,1})$.
Use $J_s(n, \theta^{k,n,2})$ to eliminate $\hat{e}_{2n,n}$ from the right. Set
$\hat{E} := \hat{E} J_s(n, \theta^{k,n,2})$,
$Q_1 := Q_1 J_s(n, \theta^{k,n,2})$.

% *Annihilate* $\hat{A}_{k+1:n,k}$.
For $j = n, n-1, \ldots, k+1$
Use $J(j-1, j, \phi^{k,j,1})$ to eliminate $\hat{a}_{j,k}$ from the left. Set
$\hat{E} := J(j-1, j, \phi^{k,j,1})^T \hat{E}$,
$\hat{A} := J(j-1, j, \phi^{k,j,1})^T \hat{A}$,
$Q_3 := Q_3 J(j-1, j, \phi^{k,j,1})$.
Use $G_s(j-1, j, \phi^{k,j,2})$, to eliminate $\hat{e}_{j,j-1}$ from the right. Set
$\hat{E} := \hat{E} G_s(j-1, j, \phi^{k,j,2})$,
$Q_1 := Q_1 G_s(j-1, j, \phi^{k,j,2})$.
Use $J(n+j-1, n+j, \phi^{k,j,3})$ to eliminate $\hat{e}_{n+j-1,n+j}$ from the left. Set
$\hat{E} := J(n+j-1, n+j, \phi^{k,j,3})^T \hat{E}$,
$\hat{A} := J(n+j-1, n+j, \phi^{k,j,3})^T \hat{A}$,
$Q_3 := Q_3 J(n+j-1, n+j, \phi^{k,j,3})$.
Endfor $j$

% *Annihilate* $\hat{A}_{n+k,k+1:n}$ *and* $\hat{A}_{n+k,n+k+2:2n}$.
Use $P_s(k+1, u^k)$ to eliminate $\hat{A}_{n+k,k+2:n}$ from the right. Set
$\hat{A} := \hat{A} P_s(k+1, u^k)$,
$Q_2 := Q_2 P_s(k+1, u^k)$.
Use $J_s(k+1, \psi^k)$ to eliminate $\hat{a}_{n+k,k+1}$ from the right. Set
$\hat{A} := \hat{A} J_s(k+1, \psi^k)$,
$Q_2 := Q_2 J_s(k+1, \psi^k)$.
Use $P_s(k+1, v^k)$ to eliminate $\hat{A}_{n+k,n+k+2:2n}$ from the right. Set
$\hat{A} := \hat{A} P_s(k+1, v^k)$,
$Q_2 := Q_2 P_s(k+1, v^k)$.
Endfor $k$

% *Annihilate* $\hat{a}_{2n,n}$.
Use $J_s(n, \theta^{n,n,1})$ to eliminate $\hat{a}_{2n,n}$ from the left. Set
$\hat{E} := J_s(n, \theta^{n,n,1})^T \hat{E}$,
$\hat{A} := J_s(n, \theta^{n,n,1})^T \hat{A}$,
$Q_3 := Q_3 J_s(n, \theta^{n,n,1})$.

Use $J_s(n, \theta^{n,n,2})$ to eliminate $\hat{e}_{2n,n}$ from the right. Set

$$\begin{aligned} \hat{E} &:= \hat{E}J_{(}n, \theta^{n,n,2}), \\ Q_1 &:= Q_1 J_s(n, \theta^{n,n,2}). \end{aligned}$$

**End**

If only the condensed form is required (i.e., the orthogonal transformations are not accumulated) then the algorithm requires about $84n^3$ flops which is less than the initial Hessenberg–triangular reduction in the standard QZ algorithm which requires $90\frac{2}{3}n^3$ flops. Although Algorithm 3 generates more zeros than the Hessenberg-triangular reduction, it is cheaper as far as the computational cost is concerned. This is due to the fact that we can apply Householder matrices to $A$ from the right during the reduction process whereas the Hessenberg-triangular reduction relies on $2 \times 2$ rotations (or reflections).

We demonstrate how the algorithm works using a $6 \times 6$ example (i.e., $n = 3$). Suppose we have reduced $E$ to triangular form and updated $A$ as in Step 1 of Algorithm 3, i.e.,

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix}.$$

The first Givens rotation $J_1 := J(n+1, n+2, \theta^{1,1,1}) = J(4, 5, \theta^{1,1,1})$ is then used to eliminate $\hat{a}_{n+1,1} = \hat{a}_{4,1}$ from the left, resulting in

$$\hat{E} := J_1^T \hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & \otimes & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := J_1^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix}.$$

We have introduced a nonzero element $\hat{e}_{n+1,n+2} = \hat{e}_{4,5}$ (denoted by $\otimes$) which is now annihilated by $G_1 := G_s(1, 2, \theta^{1,1,2})$ from the right,

$$\hat{E} := \hat{E}G_1 = \begin{bmatrix} x & x & x & x & x & x \\ \otimes & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix},$$

resulting in a nonzero element $e_{2,1}$. This is eliminated applying $J_2 := J(1, 2, \theta^{1,1,3})$ from the left,

$$\hat{E} := J_2^T \hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := J_2^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix}.$$

Thus, we have annihilated the $(n+1,1)=(4,1)$ entry of $\hat{A}$, while keeping the zero structure of $\hat{E}$. Analogously, the entries $\hat{a}_{n+j,1}$, $j=1,\ldots,n-1$, are eliminated while at the same time restoring the destroyed zeros in $\hat{E}$ such that

$$\hat{E}=\begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A}=\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ x & x & x & x & x & x \end{bmatrix}.$$

Next, the $(2n,1)=(6,1)$ entry of $\hat{A}$ is eliminated employing a Givens symplectic matrix $J_3 := J_s(n,\theta^{1,n,1}) = J_s(3,\theta^{1,3,1})$ which introduces a nonzero element in position $(2n,n)=(6,3)$ of $\hat{E}$,

$$\hat{E}:=J_3^T\hat{E}=\begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & \otimes & x & x & x \end{bmatrix}, \quad \hat{A}:=J_3^T\hat{A}=\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Now $\hat{e}_{2n,n}=\hat{e}_{6,3}$ is annihilated by applying $J_4 := J_s(n,\theta^{1,n,2}) = J_s(3,\theta^{1,3,2})$ from the right. Hence, we obtain

$$\hat{E}:=\hat{E}J_4=\begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A}=\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

To eliminate the upper part of the first column of $\hat{A}$, we use a similar sequence of transformations as for the lower part, but this time we start from the bottom element $\hat{a}_{n,1}=\hat{a}_{3,1}$ which is eliminated by using a Givens rotation $J_5 := J(n-1,n,\phi^{1,n,1}) = J(2,3,\phi^{1,3,1})$.

$$\hat{E}:=J_5^T\hat{E}=\begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & \otimes & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A}:=J_5^T\hat{A}=\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

To restore the triangular structure of $\hat{E}$, we first employ $G_2 := G_s(2,3,\phi^{1,3,2})$,

$$\hat{E}:=\hat{E}G_3=\begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & \otimes \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A}=\begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}$$

Then $\hat{e}_{5,6}$ can be eliminated using $J_6 := J(5, 6, \phi^{1,3,3})$ such that

$$\hat{E} := J_6^T \hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := J_6^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

With the same sequence of rotations we can annihilate the entries $\hat{a}_{j,1}$, $j = n-1, n-2, \ldots, 2$ (here, this is only $\hat{a}_{2,1}$) and retain the triangular structure of $\hat{E}$. We then obtain

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

The next step involves only the application of three symplectic transformations from the right to $\hat{A}$ which do not affect $\hat{E}$. First, a symplectic Householder matrix is used to annihilate $\hat{A}_{n+1,3:n} = \hat{A}_{4,3:3}$,

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := \hat{A}P_s(2, u^1) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & 0 & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Second, $\hat{a}_{n+1,2} = \hat{a}_{4,2}$ is eliminated by a symplectic Givens rotation,

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := \hat{A}J_s(2, \psi^1) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & 0 & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Last, another symplectic Householder reflection yields

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} := \hat{A}P_s(2, u^2) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

That is, we have generated the required structure in rows and columns 1 and $n+1 = 4$. In the next execution of the outer $(k)$ loop, the same sequence of transformations is used in rows and columns 2 and $n+2=5$ and we obtain

$$\hat{E} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & x & x & x & x \end{bmatrix}.$$

The final step consists of eliminating $\hat{a}_{2n,n} = \hat{a}_{6,3}$ using $J_7 := J_s(n, \theta^{n,n,1}) = J_s(3, \theta^{3,3,1})$ such that

$$\hat{E} = J_7^T \hat{E} \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & \otimes & x & x & x \end{bmatrix}, \quad \hat{A} := J_7^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x & x \end{bmatrix}$$

and then restoring the triangular structure of $\hat{E}$ by applying $J_8 := J_s(n, \theta^{n,n,1}) = J_s(3, \theta^{3,3,2})$ from the right to $\hat{E}$ which yields the desired form

$$\hat{E} := \hat{E} J_8 = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \end{bmatrix}, \quad \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x & x \end{bmatrix}.$$

Again the algorithm simplifies substantially if we have a matrix rather than a pencil.

**Algorithm 4** *Reduction of a general real $2n \times 2n$ matrix to the condensed form analogous to (6).*
**Input:** Real $2n \times 2n$ matrix $A$.
**Output:** Orthogonal matrices $Q_1, Q_2 \in \mathbf{US_{2n}}$, and transformed matrix

$$\hat{A} \ := \ Q_1^T A Q_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}$$

where $A_{ij} \in \mathbf{R}^{n \times n}$, $A_{11}$ is upper triangular and $A_{22}^T$ is upper Hessenberg.

Set $\hat{A} \ := \ A, \qquad Q_1 \ := \ I_{2n}, \qquad Q_2 \ := \ I_{2n}.$
For $k = 1, \ldots, n-1$
% *Annihilate* $\hat{A}_{k+1:2n,k}$.
Use $P_s(k, u^{k,1})$ to eliminate $\hat{A}_{n+k+1:2n,k}$ from the left. Set
$\hat{A} \ := \ P_s(k, u^{k,1}) \hat{A}$,
$Q_1 \ := \ Q_1 P_s(k, u^{k,1})$.
Use $J_s(k, \theta^k)$ to eliminate $\hat{a}_{n+k,k}$ from the left. Set
$\hat{A} \ := \ J_s(k, \theta^k)^T \hat{A}$,
$Q_1 \ := \ Q_1 J_s(k, \theta^k)$.

Use $P_s(k, u^{k,2})$ to eliminate $\hat{A}_{k+1:n,k}$ from the left. Set

$$\begin{aligned} \hat{A} &:= P_s(k, u^{k,2})\hat{A}, \\ Q_1 &:= Q_1 P_s(k, u^{k,2}). \end{aligned}$$

% *Annihilate* $\hat{A}_{n+k,k+1:n}$ *and* $\hat{A}_{n+k,n+k+2:2n}$.

Use $P_s(k+1, v^{k,1})$ to eliminate $\hat{A}_{n+k,k+2:n}$ from the right. Set

$$\begin{aligned} \hat{A} &:= \hat{A}P_s(k+1, v^{k,1}), \\ Q_2 &:= Q_2 P_s(k+1, v^{k,1}). \end{aligned}$$

Use $J_s(k+1, \phi^k)$ to eliminate $\hat{a}_{n+k,k+1}$ from the right. Set

$$\begin{aligned} \hat{A} &:= \hat{A}J_s(k+1, \phi^k), \\ Q_2 &:= Q_2 J_s(k+1, \phi^k). \end{aligned}$$

Use $P_s(k+1, v^{k,2})$ to eliminate $\hat{A}_{n+k,n+k+2:2n}$ from the right. Set

$$\begin{aligned} \hat{A} &:= \hat{A}P_s(k+1, v^{k,2}), \\ Q_2 &:= Q_2 P_s(k+1, v^{k,2}). \end{aligned}$$

Endfor $k$

% *Annihilate* $\hat{a}_{2n,n}$.

Use $J_s(n, \theta^n)$ to eliminate $\hat{a}_{2n,n}$ from the left. Set

$$\begin{aligned} \hat{A} &:= J_s(n, \theta^n)^T \hat{A}, \\ Q_1 &:= Q_1 J_s(n, \theta^n). \end{aligned}$$

End

If only eigenvalues are required, the orthogonal transformations need not be accumulated. In that case, Algorithm 4 requires $80n^3/3 + 20n^2$ flops. This is comparable to reducing the Hamiltonian matrix to Hessenberg form by Householder reflections which requires $80n^3/3 - 10n^2$ flops. That is, the initial reductions necessary for either Algorithm 2 or the standard Hessenberg QR algorithm are equally expensive as far as floating point operations are concerned. Besides the $O(n^2)$ difference in the flop count, Algorithm 4 is more complicated than the standard Householder Hessenberg reduction as far as indexing, subroutine calls, and updating the transformations are concerned. This will in practise lead to a slightly higher execution time than for the Householder Hessenberg reduction.

We will illustrate the reduction of a $2n \times 2n$ to the condensed form (6) using a $6 \times 6$ example. First, we have to annihilate the first column of $A$. Using a symplectic Householder reflection we can eliminate all entries below the diagonal in the first column of the lower left block of $A$.

$$\hat{A} := P_s(1, u^{1,1})A = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

The entry in position $(n+1, 1) = (4, 1)$ is then eliminated using a symplectic Givens rotation such that

$$\hat{A} := J_s(1, \theta^1)^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ x & x & x & x & x & x \\ x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Now the elements below the diagonal of the upper left block of $\hat{A}$ are annihilated using again a symplectic Householder reflection.

$$\hat{A} := P_s(1, u^{1,2})A = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

The next three steps reduce the $(n+1)$st $= 4$th row of $\hat{A}$ to the desired form. Applying a symplectic Householder reflection form the right, we can annihilate $\hat{A}_{n+1,3:n} = \hat{A}_{4,3:3}$, resulting in

$$\hat{A} := \hat{A}P_s(2, v^{1,1}) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & 0 & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Then, $\hat{a}_{n+1,2} = \hat{a}_{4,2}$ is eliminated by a symplectic Givens rotation,

$$\hat{A} := \hat{A}J_s(2, \phi^1) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & 0 & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

Next, another symplectic Householder reflection yields

$$\hat{A} := \hat{A}P_s(2, v^{1,2}) = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & x & x & x & x & x \\ 0 & x & x & x & x & x \end{bmatrix}.$$

That is, we have generated the required structure in rows and columns 1 and $n+1 = 4$. In the next execution of the outer loop, the same sequence of transformations is used in rows and columns 2 and $n+2 = 5$ and we obtain

$$\hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & x & x & x & x \end{bmatrix}.$$

The final step consists of eliminating $\hat{a}_{2n,n} = \hat{a}_{6,3}$ using $J_s(3, \theta^3)$ such that

$$\hat{A} := J_s(3, \theta^3)^T \hat{A} = \begin{bmatrix} x & x & x & x & x & x \\ 0 & x & x & x & x & x \\ 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & x & x & 0 \\ 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x & x \end{bmatrix}.$$

# 5 Error Analysis

In this section, we will derive the error analysis for Algorithms 1 and 2.

Since in both methods all transformations are performed with orthogonal and orthogonal symplectic matrices we can apply the standard backward error analysis of Wilkinson, e.g. [27, 9]. To do this we need to analyse the backward error. We begin with an analysis of the computation of the eigenvalues of a Hamiltonian matrix $\mathcal{H}$ via Algorithm 2.

Using the usual arguments in the analysis of orthogonal transformations, e.g., [27, 9], we obtain that there exists a $2n \times 2n$ matrix $E$, with $\|E\| \leq \varepsilon \|\mathcal{H}\|$, where $\varepsilon$ is a small number equivalent to the machine precision, and $\hat{Q}_1, \hat{Q}_2 \in \mathbf{US_{2n}}$ such that the computed factorization satisfies

$$\hat{\mathcal{H}} := \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} = \hat{Q}_1^T (\mathcal{H} + E) \hat{Q}_2. \tag{41}$$

Note that if $\hat{\lambda}$ is a computed eigenvalue of $\mathcal{H}$, we have that $\hat{\lambda}^2$ is an eigenvalue of

$$\begin{bmatrix} -H_{22}^T & H_{12}^T \\ 0 & -H_{11}^T \end{bmatrix} \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} = J\hat{\mathcal{H}}^T J\hat{\mathcal{H}},$$

and by (41) $\hat{\lambda}^2$ is also an eigenvalue of $(\mathcal{H} + JE^T J)(\mathcal{H} + E)$.

The *condition* of a simple eigenvalue $\lambda$ of a matrix $A \in \mathbf{R}^{n \times n}$ as defined in [27] is given by

$$\frac{1}{s(\lambda)} = \frac{1}{|y^H x|} \tag{42}$$

where $x$ and $y$ with $\|x\|_2 = \|y\|_2 = 1$ are the right and left, respectively, eigenvectors of $A$ corresponding to $\lambda$.

**Theorem 9** *Let $\lambda$ be a nonzero and simple eigenvalue of a real Hamiltonian matrix $\mathcal{H} \in \mathbf{H_{2n}}$, and let $1/s(\lambda)$ be its condition number as given in (42). Let $\varepsilon$ be the machine precision. If the matrix $E$ in (41) satisfies $\|E\| < \varepsilon \|\mathcal{H}\|$, and $\frac{2\|\mathcal{H}\|\varepsilon}{|\lambda| s(\lambda)} < 1$, then Algorithm 2 yields a computed eigenvalue $\hat{\lambda}$ such that*

$$|\hat{\lambda} - \lambda| \leq \frac{\|\mathcal{H}\|\,\varepsilon}{(1 - \frac{\|\mathcal{H}\|\varepsilon}{|\lambda| s(\lambda)}) s(\lambda)} + O(\varepsilon^2) \leq \frac{2\,\|\mathcal{H}\|\,\varepsilon}{s(\lambda)} + O(\varepsilon^2). \tag{43}$$

*Proof.* Since we have assumed that $\lambda$ is simple, from Lemma 3 b) we obtain that $\lambda^2$ is a nondefective eigenvalue of $\mathcal{H}^2$ of multiplicity two. Furthermore, if $y$, $x$ with $\|x\| = 1$, $\|y\| = 1$ are the left and right eigenvectors of $\mathcal{H}$ to $\lambda$ then they are also eigenvectors of $\mathcal{H}^2$ to the eigenvalue $\lambda^2$.

Now consider perturbations in the matrix $(\mathcal{H} + JE^TJ)(\mathcal{H} + E)$. Clearly

$$(\mathcal{H} + JE^TJ)(\mathcal{H} + E) = \mathcal{H}^2 + \mathcal{H}E + JE^TJ\mathcal{H} + JE^TJE, \tag{44}$$

which is $\mathcal{H}^2$ perturbed with a matrix of order $O(\varepsilon)$. From the analytical properties of simple eigenvalues and its eigenvectors and the discussions given above, it follows that when $\varepsilon$ is sufficiently small, there exists an eigenvalue $\hat{\lambda}^2$ of $(\mathcal{H} + JE^TJ)(\mathcal{H} + E)$, such that its unit left and right eigenvectors $\hat{y}$, $\hat{x}$ can be expanded as $\hat{y} = y + \varepsilon y_1 + O(\varepsilon^2)$, $\hat{x} = x + \varepsilon x_1 + O(\varepsilon^2)$. Multiplying by $y^H$ on the left and by $x$ on the right hand sides of (44), and using $y^H\mathcal{H} = \lambda y^H$, $\mathcal{H}x = \lambda x$, we obtain

$$\begin{aligned} y^H(\mathcal{H} + JE^TJ)(\mathcal{H} + E)x &= y^H(\mathcal{H}^2 + \mathcal{H}E + JE^TJ\mathcal{H} + JE^TJE)x \\ &= \lambda^2 y^H x + \lambda y^H(E + JE^TJ)x + O(\varepsilon^2). \end{aligned}$$

On the other hand,

$$\begin{aligned} y^H(\mathcal{H} + JE^TJ)(\mathcal{H} + E)x &= \left(\hat{y}^H - \varepsilon y_1^H + O(\varepsilon^2)\right)(\mathcal{H} + JE^TJ)(\mathcal{H} + E)\left(\hat{x} - \varepsilon x_1 + O(\varepsilon^2)\right) \\ &= \hat{\lambda}^2\left(\hat{y}^H\hat{x} - \varepsilon(\hat{y}^H x_1 + y_1^H\hat{x})\right) + O(\varepsilon^2) \\ &= \hat{\lambda}^2 y^H x + O(\varepsilon^2). \end{aligned}$$

Therefore

$$\hat{\lambda}^2 - \lambda^2 = \frac{\lambda y^H(E + JE^TJ)x}{y^H x} + O(\varepsilon^2),$$

and with the reciprocal eigenvalue condition number $s(\lambda) = |y^H x|$, we obtain

$$|\hat{\lambda} + \lambda|\,|\hat{\lambda} - \lambda| \le \frac{2\,\|\mathcal{H}\|\,|\lambda|\varepsilon}{s(\lambda)} + O(\varepsilon^2). \tag{45}$$

Using the inequality $|\hat{\lambda} + \lambda| > 2|\lambda| - |\hat{\lambda} - \lambda|$ together with the inequality $\frac{2\|\mathcal{H}\|\varepsilon}{|\lambda|s(\lambda)} < 1$ and omitting the second order perturbations, we obtain (43) by solving the quadratic inequality

$$|\hat{\lambda} - \lambda|^2 - 2|\lambda|\,|\hat{\lambda} - \lambda| + \frac{2\,\|\mathcal{H}\|\,|\lambda|\varepsilon}{s(\lambda)} \ge 0.$$

□

As a consequence of Theorem 9 we have that Algorithm 2 is numerically backward stable.

**Remark 6** From the error analysis in Theorem 9 we see the major difference between the new method and the square reduced method of Van Loan for which the perturbation analysis yields that the computed eigenvalues are the exact eigenvalues of $\mathcal{H}^2 + F$, and the perturbation satisfies $\|F\| < \varepsilon\,\|\mathcal{H}^2\|$. In our new approach we can avoid squaring the matrix, but as we have seen in Section 4, the prize is an increase in computational cost.

Now we give an error analysis for the eigenvalues of a Hamiltonian pencil.

Let $(\lambda, 1)$ be a nonzero finite simple eigenvalue of a real regular Hamiltonian pencil $\alpha\mathcal{E} - \beta\mathcal{A}$, then by Proposition 1 a), $(-\lambda, 1)$ is also a simple eigenvalue of $\alpha\mathcal{E} - \beta\mathcal{A}$. Furthermore, if $y$, $x$ with $\|y\|, \|x\| = 1$ are the left eigenvectors corresponding to $(\lambda, 1)$ and $(-\lambda, 1)$, respectively, then we have

$$y^H(\lambda\mathcal{E} - \mathcal{A}) = 0, \qquad (\lambda\mathcal{E} - \mathcal{A})J\mathcal{E}^T\bar{x} = 0; \tag{46}$$

$$x^H(-\lambda\mathcal{E}-\mathcal{A})=0, \qquad (-\lambda\mathcal{E}-\mathcal{A})J\mathcal{E}^T\bar{y}=0. \tag{47}$$

If we take the *chordal distance* (see [24, page 283]) as a metric for the complex numbers, i.e.,

$$\chi((\alpha,\beta),(\gamma,\delta))=\frac{|\alpha\delta-\beta\gamma|}{\sqrt{|\alpha|^2+|\beta|^2}\sqrt{|\gamma|^2+|\delta|^2}}$$

then the condition numbers of $(\lambda,1)$ and $(-\lambda,1)$ are [9, 24]

$$\kappa(\lambda) := \frac{\left\|\mathcal{E}^T\bar{x}\right\|}{\sqrt{|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|^2+|y^H\mathcal{A}J\mathcal{E}^T\bar{x}|^2}}, \tag{48}$$

$$\kappa(-\lambda) := \frac{\left\|\mathcal{E}^T\bar{y}\right\|}{\sqrt{|x^H\mathcal{E}J\mathcal{E}^T\bar{y}|^2+|x^H\mathcal{A}J\mathcal{E}^T\bar{y}|^2}}. \tag{49}$$

Since $\mathcal{E}J\mathcal{A}^T=-\mathcal{A}J\mathcal{E}^T=\mathcal{A}J^T\mathcal{E}^T$ we have

$$\begin{aligned}\alpha^2\mathcal{E}J\mathcal{E}^T-\beta^2\mathcal{A}J^T\mathcal{A}^T &= (\alpha\mathcal{E}-\beta\mathcal{A})J(\alpha\mathcal{E}-\beta\mathcal{A})^T\\ &= (\alpha\mathcal{E}+\beta\mathcal{A})J(\alpha\mathcal{E}+\beta\mathcal{A})^T.\end{aligned}$$

It is clear that $(\lambda^2,1)$ is a double eigenvalue of $\alpha\mathcal{E}J\mathcal{E}^T-\beta\mathcal{A}J^T\mathcal{A}^T$, and

$$y^H(\lambda^2\mathcal{E}J\mathcal{E}^T-\mathcal{A}J^T\mathcal{A}^T)=0, \qquad (\lambda^2\mathcal{E}J\mathcal{E}^T-\mathcal{A}J^T\mathcal{A}^T)\bar{x}=0 \tag{50}$$

which means that $y$ and $\bar{x}$ are left and right eigenvectors of $\alpha\mathcal{E}J\mathcal{E}^T-\beta\mathcal{A}J^T\mathcal{A}^T$ corresponding to $(\lambda^2,1)$.

Similar to the matrix case, the eigenvalue $(\hat{\lambda}^2,1)$, where $(\hat{\lambda},1)$ is computed by Algorithm 1, can be considered as an eigenvalue of the matrix pencil

$$\alpha(\mathcal{E}+E)J(\mathcal{E}+E)^T-\beta(\mathcal{A}+F)J^T(\mathcal{A}+F)^T,$$

where $E$ and $F$ are real small perturbation matrices satisfying

$$\|[E,\ F]\|\le\varepsilon\,\|[\mathcal{E},\ \mathcal{A}]\| \tag{51}$$

(see [9, 19]). We then get

**Theorem 10** *Let $(\lambda,1)$ be a nonzero simple eigenvalue of a real regular Hamiltonian pencil $\alpha\mathcal{E}-\beta\mathcal{A}$. If*

$$\frac{\sqrt{1+|\lambda|^2}}{|\lambda|}\frac{\left(\left\|\mathcal{E}^T\bar{y}\right\|+\left\|\mathcal{E}^T\bar{x}\right\|\right)}{y^H\mathcal{E}J\mathcal{E}^T\bar{x}}\,\|[\mathcal{E},\ \mathcal{A}]\|\,\varepsilon<1 \tag{52}$$

*where $y$, $x$ are defined in (46), (47), and if we set $\kappa(\lambda,-\lambda):=\kappa(\lambda)+\kappa(-\lambda)$ where $\kappa(\lambda)$ and $\kappa(-\lambda)$ are defined as in (48) and (49), then there is an eigenvalue $(\hat{\lambda},1)$ computed by Algorithm 1 such that*

$$\chi((\hat{\lambda},1),(\lambda,1))\le\varepsilon\,\|[\mathcal{E},\ \mathcal{A}]\|\,\kappa(\lambda,-\lambda)+O(\varepsilon^2). \tag{53}$$

*Proof.* If $(\hat{\lambda}, 1)$ is the analogue of $(\lambda, 1)$, computed by Algorithm 1, then $(\hat{\lambda}^2, 1)$ is an exact eigenvalue of the matrix pencil

$$\alpha(\mathcal{E}+E)J(\mathcal{E}+E)^T - \beta(\mathcal{A}+F)J^T(\mathcal{A}+F)^T$$

with $E, F \in \mathbf{R}^{2n\times 2n}$ satisfying (51), i.e., $\|[E,\ F]\| \le \varepsilon \,\|[\mathcal{E},\ \mathcal{A}]\|$. This matrix pencil can be considered as the pencil $\alpha\mathcal{E}J\mathcal{E}^T - \beta\mathcal{A}J^T\mathcal{A}^T$ plus a perturbation of order $\varepsilon$. Thus, from (50) and by using the result in [24, Theorem 2.2, p.293] we obtain

$$(\hat{\lambda}^2, 1) = \left( \frac{y^H(\mathcal{A}+F)J^T(\mathcal{A}+F)^T\bar{x}}{y^H(\mathcal{E}+E)J(\mathcal{E}+E)^T\bar{x}}, 1 \right) + O(\varepsilon^2). \tag{54}$$

From (46), (47), and (50) we get

$$y^H(\mathcal{A}+F)J^T(\mathcal{A}+F)^T\bar{x} = \lambda^2 y^H\mathcal{E}J\mathcal{E}^T\bar{x} - \lambda(y^H\mathcal{E}JF^T\bar{x} - y^HFJ\mathcal{E}^T\bar{x}) + O(\varepsilon^2)$$

and

$$y^H(\mathcal{E}+E)J(\mathcal{E}+E)^T\bar{x} = y^H\mathcal{E}J\mathcal{E}^T\bar{x} + y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x} + O(\varepsilon^2).$$

(Note that by assumption (52) and without considering the $O(\varepsilon^2)$ terms,

$$|y^H(\mathcal{E}+E)J(\mathcal{E}+E)^T\bar{x}| \ge |y^H\mathcal{E}J\mathcal{E}^T\bar{x}| - \varepsilon(\left\|\mathcal{E}^T\bar{y}\right\| + \left\|\mathcal{E}^T\bar{x}\right\|)\,\|[\mathcal{E},\ \mathcal{A}]\| > 0$$

and hence, the right-hand side of (54) is well defined.)

Therefore

$$\begin{aligned}
\hat{\lambda}^2 y^H(\mathcal{E}+E)J(\mathcal{E}+E)^T\bar{x} - y^H(\mathcal{A}+F)J^T(\mathcal{A}+F)^T\bar{x} &= \\
(\hat{\lambda}^2-\lambda^2)y^H\mathcal{E}J\mathcal{E}^T\bar{x} + \hat{\lambda}^2(y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}) & \\
+\ \lambda(y^H\mathcal{E}JF^T\bar{x} - y^HFJ\mathcal{E}^T\bar{x}) &= \\
(\hat{\lambda}^2-\lambda^2)(y^H\mathcal{E}J\mathcal{E}^T\bar{x} + y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}) & \\
+\ \lambda^2(y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}) + \lambda(y^H\mathcal{E}JF^T\bar{x} - y^HFJ\mathcal{E}^T\bar{x}) &= O(\varepsilon^2)
\end{aligned}$$

Hence, by omitting the second order terms, we have

$$\begin{aligned}
\lambda^2 - \hat{\lambda}^2 &\approx \frac{\lambda^2(y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}) + \lambda(y^H\mathcal{E}JF^T\bar{x} - y^HFJ\mathcal{E}^T\bar{x})}{y^H\mathcal{E}J\mathcal{E}^T\bar{x} + y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}} \\
&\approx \frac{\lambda\left\{\lambda(y^H\mathcal{E}JE^T\bar{x} + y^HEJ\mathcal{E}^T\bar{x}) + y^H\mathcal{E}JF^T\bar{x} - y^HFJ\mathcal{E}^T\bar{x}\right\}}{y^H\mathcal{E}J\mathcal{E}^T\bar{x}.}
\end{aligned}$$

Thus,

$$\begin{aligned}
|\hat{\lambda}-\lambda||\hat{\lambda}+\lambda| &\simeq \frac{|\lambda| \left( \left| [\lambda y^H\mathcal{E}J,\ y^H\mathcal{E}J] \begin{bmatrix} E^T \\ F^T \end{bmatrix} \bar{x} + y^H[E,\ F] \begin{bmatrix} \lambda J\mathcal{E}^T\bar{x} \\ -J\mathcal{E}^T\bar{x} \end{bmatrix} \right| \right)}{|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|} \\
&\le \frac{|\lambda|\sqrt{1+|\lambda|^2}\,\|[E,\ F]\|\,(\left\|\mathcal{E}^T\bar{y}\right\| + \left\|\mathcal{E}^T\bar{x}\right\|)}{|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|.}
\end{aligned}$$

By using the condition

$$\frac{\varepsilon\sqrt{1+|\lambda|^2}\,\|[\mathcal{E},\ \mathcal{A}]\|\,(\left\|\mathcal{E}^T\bar{y}\right\|+\left\|\mathcal{E}^T\bar{x}\right\|)}{|\lambda||y^H\mathcal{E}J\mathcal{E}^T\bar{x}|}<1$$

and $|\hat{\lambda}+\lambda|\geq 2|\lambda|-|\hat{\lambda}-\lambda|$, we get

$$|\hat{\lambda}-\lambda|<\frac{\varepsilon\sqrt{1+|\lambda|^2}\,\|[\mathcal{E},\ \mathcal{A}]\|\,(\left\|\mathcal{E}^T\bar{y}\right\|+\left\|\mathcal{E}^T\bar{x}\right\|)}{|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|}.$$

From (46) we have

$$\lambda y^H\mathcal{E}J\mathcal{E}^T\bar{x}=y^H\mathcal{A}J\mathcal{E}^T\bar{x},$$

and thus

$$(1+|\lambda|^2)|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|^2=|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|^2+|y^H\mathcal{A}J\mathcal{E}^T\bar{x}|^2$$

Finally we get

$$\begin{aligned}
\chi((\lambda,1),(\hat{\lambda},1)) &= \frac{|\lambda-\hat{\lambda}|}{\sqrt{1+|\lambda|^2}\sqrt{1+|\hat{\lambda}|^2}}\\
&\simeq \frac{|\lambda-\hat{\lambda}|}{1+|\lambda|^2}\\
&< \frac{\varepsilon\,\|[\mathcal{E},\ \mathcal{A}]\|\,(\left\|\mathcal{E}^T\bar{y}\right\|+\left\|\mathcal{E}^T\bar{x}\right\|)}{\sqrt{1+|\lambda|^2}|y^H\mathcal{E}J\mathcal{E}^T\bar{x}|}\\
&= \varepsilon\,\|[\mathcal{E},\ \mathcal{A}]\|\,\kappa(\lambda,-\lambda),
\end{aligned}$$

which proves (53). □

**Remark 7** Clearly, the bound (53) also holds for the eigenvalue $(-\lambda,1)$.

**Remark 8** Usually $\kappa(\lambda)$ and $\kappa(-\lambda)$ are different and thus, the eigenvalue condition number $\kappa(\lambda,-\lambda)\leq 2\max\{\kappa(\lambda),\kappa(-\lambda)\}$ is a combination of $\kappa(\lambda)$ and $\kappa(-\lambda)$. This is the condition number of our method both for $(\lambda,1)$ and $(-\lambda,1)$. If we consider structured perturbations, i.e., $E$, $F$ with $\|[E\ F]\|<\varepsilon\,\|[\mathcal{E},\ \mathcal{A}]\|$ such that $\alpha(\mathcal{E}+E)-\beta(\mathcal{A}+F)$ is still a Hamiltonian pencil, then $\kappa(\lambda)\approx\kappa(-\lambda)$ In this case, $(\lambda,1)$ and $(-\lambda,1)$ have equivalent perturbation properties. So we can assume that in general $\kappa(\lambda)$ and $\kappa(-\lambda)$ have the same magnitude. If this is true, then the bound (53) is as good as the standard perturbation bound.

## 6 Numerical Examples

Algorithm 2 was implemented in Fortran 77 and was tested for all examples given in the benchmark collections for continuous-time algebraic Riccati equations [5], the examples given in [25], and some randomly generated examples. Here, we present the most interesting results obtained by these experiments.

The numerical tests were performed using IEEE double precision arithmetic with machine precision $\varepsilon\approx 2.2204\times 10^{-16}$ on a HP Model 712/60 workstation with operating system HP-UX 9.0. As compiler we used the HP-UX Fortran 77 compiler as invoked by `f77`. The programs were compiled using only minimal optimization.

We compared the following methods:

- **URVHQR**, the symplectic URV decomposition given in Algorithm 4 and Hessenberg QR iteration using LAPACK subroutine DHSEQR, i.e., the product $-H_{22}^T H_{11}$ was formed explicitly,
- **URVPSD**, the symplectic URV decomposition given in Algorithm 4 and the periodic Schur decomposition [10] as implemented in [26],
- **SQRED**, Van Loan's square reduced method as implemented in [4],
- **LAPACK**, nonsymmetric eigenproblem solver DGEEVX from LAPACK [3].

All subroutines use the BLAS and LAPACK [3] as far as possible.

**Example 2** [25, Example 2] Let

$$F = \mathrm{diag}(1,\, 10^{-2},\, 10^{-4},\, 10^{-6},\, 10^{-8}\,)$$

then a Hamiltonian matrix $\mathcal{H}$ is obtained by

$$\mathcal{H} = \mathcal{U}^T \begin{bmatrix} F & 0 \\ 0 & -F^T \end{bmatrix} \mathcal{U},$$

with $\mathcal{U} \in \mathbf{US_{2n}}$ randomly generated by five symplectic rotations and five reflectors. Thus,

$$\sigma(\mathcal{H}) = \{\pm 1, \pm 10^{-2}, \pm 10^{-4}, \pm 10^{-6}, \pm 10^{-8}\}.$$

Table 1 shows the absolute errors in the eigenvalue approximations computed by the four methods.

| $\lambda$ | URVHQR | URVPSD | SQRED | LAPACK |
|---|---|---|---|---|
| 1 | 0 | 0 | 0 | $7.8 \times 10^{-16}$ |
| $10^{-2}$ | $5.5 \times 10^{-16}$ | $5.5 \times 10^{-16}$ | $5.5 \times 10^{-16}$ | $5.0 \times 10^{-17}$ |
| $10^{-4}$ | $7.7 \times 10^{-14}$ | $1.6 \times 10^{-18}$ | $1.6 \times 10^{-14}$ | $2.6 \times 10^{-18}$ |
| $10^{-6}$ | $4.1 \times 10^{-12}$ | $1.0 \times 10^{-18}$ | $1.5 \times 10^{-11}$ | $8.4 \times 10^{-18}$ |
| $10^{-8}$ | $1.7 \times 10^{-9}$ | $3.1 \times 10^{-17}$ | $2.2 \times 10^{-9}$ | $4.7 \times 10^{-17}$ |

Table 1: Example 2, absolute errors $|\lambda - \tilde{\lambda}|$

From Table 1 the loss of accuracy of $\|H\| / |\lambda|$ for Van Loan's method is obvious. The same loss of accuracy is observed as was to be expected when the symplectic URV decomposition is used but the product $-H_{22}^T H_{11}$ is formed explicitly. Using the periodic Schur decomposition yields the exact eigenvalues with respect to machine precision as does the QR algorithm implemented in LAPACK.

**Example 3** [25, Example 3] The Frank matrix $F \in \mathbf{R}^{n\times n}$ is defined by

$$F = \begin{bmatrix} n & n-1 & n-2 & \dots & \dots & 2 & 1 \\ n-1 & n-1 & n-2 & \dots & \dots & 2 & 1 \\ 0 & n-2 & n-2 & \dots & \dots & 2 & 1 \\ 0 & 0 & n-3 & \ddots & & \vdots & \vdots \\ \vdots & \vdots & & \ddots & \ddots & \vdots & \vdots \\ \vdots & \vdots & & & \ddots & 2 & 1 \\ 0 & 0 & \dots & & 0 & 1 & 1 \end{bmatrix}.$$

All the eigenvalues are real and positive. For increasing $n$, the eigenvalue condition number becomes worse for the small eigenvalues. A Hamiltonian matrix having the same eigenvalues as the Frank matrix together with their negative counterparts is generated as in Example 2,

$$\mathcal{H} = \mathcal{U}^T \begin{bmatrix} F & 0 \\ 0 & -F^T \end{bmatrix} \mathcal{U},$$

with $\mathcal{U} \in \mathbf{US_{2n}}$ randomly generated by $n$ symplectic rotations and $n$ reflectors.

We tested all four methods for $n = 12$. Since exact eigenvalues are not known, we compare the values computed by URVHQR, URVPSD, and SQRED with those obtained by DGEEVX (denoted by $\lambda^{QR}$). The results for the five eigenvalues of smallest absolute value (and worst condition number) are shown in Table 2. (Here, $\tilde{\lambda}$ denotes the computed values by either of the three methods other than LAPACK.)

| $\lambda \approx$ | $s(\lambda)$ | URVHQR | URVPSD | SQRED |
|---|---|---|---|---|
| 0.2847 | $1.8 \times 10^{-6}$ | $1.8 \times 10^{-9}$ | $2.7 \times 10^{-11}$ | $2.8 \times 10^{-9}$ |
| 0.1436 | $1.8 \times 10^{-6}$ | $2.7 \times 10^{-8}$ | $9.9 \times 10^{-10}$ | $7.6 \times 10^{-8}$ |
| 0.08122 | $3.8 \times 10^{-8}$ | $1.4 \times 10^{-7}$ | $5.9 \times 10^{-9}$ | $5.6 \times 10^{-7}$ |
| 0.0495 | $2.6 \times 10^{-8}$ | $2.3 \times 10^{-7}$ | $9.8 \times 10^{-9}$ | $1.4 \times 10^{-6}$ |
| 0.03102 | $5.5 \times 10^{-8}$ | $1.2 \times 10^{-7}$ | $5.0 \times 10^{-9}$ | $1.1 \times 10^{-6}$ |

Table 2: Example 3, $|\tilde{\lambda} - \lambda^{QR}|$

Again, the symplectic URV decomposition yields eigenvalue approximations according to the accuracy to be expected by $s(\lambda)$ and Theorem 9 whereas both SQRED and URVHQR again loose accuracy of order $\|H\|/|\lambda|$.

**Example 4** We tested the four methods for randomly generated Hamiltonian matrices with entries distributed normally in the interval $[-1, 1]$. Since the eigenvalue distribution for these examples usually behaves nicely, the eigenvalues computed by either of the four methods are computed to almost the same accuracy. We give the CPU times for $2n \times 2n$ examples for several sizes of $n$. For each size of $n$, we computed 100 examples. The values given in Table 3 are the mean values of the CPU times measured on a HP Model 712/60 work station.

Table 3 shows that both URVHQR and SQRED are much faster than the standard QR algorithm. The speed up expected from the flop counts is not attained, though. This is due

| $n$ | URVHQR | URVPSD | SQRED | LAPACK |
|---|---|---|---|---|
| 25 | 0.045 | 0.173 | 0.052 | 0.118 |
| 50 | 0.35 | 1.13 | 0.31 | 0.71 |
| 75 | 1.13 | 3.40 | 0.95 | 2.21 |
| 100 | 2.78 | 7.99 | 2.31 | 5.01 |
| 125 | 5.42 | 15.00 | 4.53 | 9.75 |
| 150 | 9.41 | 25.53 | 7.71 | 17.25 |
| 175 | 15.18 | 40.61 | 12.22 | 28.15 |
| 200 | 22.93 | 60.24 | 18.38 | 42.45 |

Table 3: Example 4, CPU times

to the fact that both methods are more complex as far as index handling, memory access, and subroutine calls are concerned.

The CPU times for URVPSD are unsatisfactory. This is due to the high CPU times required by the implemented subroutines for the periodic Schur decomposition and are not in accordance with the flop counts — even if the abovementioned effects are taken into account.

Besides the faster computation of the eigenvalues, both URV based methods and Van Loan's method return the right pairing of the eigenvalues as $\pm\lambda_i$, $i = 1, \ldots, n$. Since DGEEVX treats a Hamiltonian matrix like an arbitrary unsymmetric matrix, small perturbations can cause computed eigenvalues with small real parts to cross the imaginary axis. For instance, the number of stable eigenvalues in Example 4 returned by DGEEVX for $n = 100$ varied between 96 and 106.

## 7 Conclusions

We have presented a new method for computing the eigenvalues of Hamiltonian matrices and pencils which can also be used for symplectic matrices and pencils employing a Cayley transformation. The method is numerically strongly backward stable, since it preserves the underlying Hamiltonian structure and uses only backward stable orthogonal transformations. The algorithms save a significant amount of computational cost compared to the standard QR and QZ algorithms. On the other hand, the new method is more expensive in both computational cost and work space than Van Loan's method and its analogues for the symplectic case, but does not suffer from the $O(\sqrt{\varepsilon})$ loss of accuracy as these methods do.

Future work will include an LAPACK-based implementation of Algorithms 1. Our algorithms strongly depend upon the performance of the periodic QR and QZ algorithms. Thus, in order to obtain reasonable execution times for Algorithms 1 and 2, excellent implementations of the periodic QR and QZ algorithm will be required.

## References


[1] G.S. Ammar, P. Benner, and V. Mehrmann. A multishift algorithm for the numerical solution of algebraic Riccati equations. *Electr. Trans. Num. Anal.*, 1:33–48, 1993.

[2] G.S. Ammar and V. Mehrmann. On Hamiltonian and symplectic Hessenberg forms. *Linear Algebra Appl.*, 149:55–72, 1991.

[3] E. Anderson, Z. Bai, C. Bischof, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, S. Ostrouchov, and D. Sorensen. *LAPACK Users' Guide.* SIAM, Philadelphia, PA, second edition, 1994.

[4] E. Barth, R. Byers, and P. Benner. HAMEV and SQRED: Fortran 77 subroutines for computing the eigenvalues of Hamiltonian matrices using Van Loan's square reduced method. preprint, Fak. f. Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG, 1996. In preparation.

[5] P. Benner, A. Laub, and V. Mehrmann. A collection of benchmark examples for the numerical solution of algebraic Riccati equations I: Continuous-time case. Technical Report SPC 95_22, Fak. f. Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG, 1995.

[6] A. Bojanczyk, G.H. Golub, and P. Van Dooren. The periodic Schur decomposition; algorithms and applications. In *Proc. SPIE Conference, vol. 1770*, pages 31–42, 1992.

[7] A. Bunse-Gerstner. Matrix factorization for symplectic QR-like methods. *Linear Algebra Appl.*, 83:49–77, 1986.

[8] A. Bunse-Gerstner, R. Byers, and V. Mehrmann. Numerical methods for algebraic Riccati equations. In S. Bittanti, editor, *Proc. Workshop on the Riccati Equation in Control, Systems, and Signals*, pages 107–116, Como, Italy, 1989.

[9] G.H. Golub and C.F. Van Loan. *Matrix Computations.* Johns Hopkins University Press, Baltimore, second edition, 1989.

[10] J.J. Hench and A.J. Laub. An extension of the QR algorithm for a sequence of matrices. Technical Report CCEC-92-0829, ECE Dept., University of California, Santa Barbara, CA, 1992.

[11] J.J. Hench and A.J. Laub. Numerical solution of the discrete-time periodic Riccati equation. *IEEE Trans. Automat. Control*, 39:1197–1210, 1994.

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

[13] A.J. Laub. A Schur method for solving algebraic Riccati equations. *IEEE Trans. Automat. Control*, AC-24:913–921, 1979. (see also *Proc. 1978 CDC (Jan. 1979)*, pp. 60-65).

[14] A.J. Laub. Algebraic aspects of generalized eigenvalue problems for solving Riccati equations. In C.I. Byrnes and A. Lindquist, editors, *Computational and Combinatorial Methods in Systems Theory*, pages 213–227. Elsevier (North-Holland), 1986.

[15] A.J. Laub. Invariant subspace methods for the numerical solution of Riccati equations. In S. Bittanti, A.J. Laub, and J.C. Willems, editors, *The Riccati Equation*, pages 163–196. Springer-Verlag, Berlin, 1991.

[16] W.-W. Lin. A new method for computing the closed loop eigenvalues of a discrete-time algebraic Riccati equation. *Linear Algebra Appl.*, 6:157–180, 1987.

[17] V. Mehrmann. *The Autonomous Linear Quadratic Control Problem, Theory and Numerical Solution.* Number 163 in Lecture Notes in Control and Information Sciences. Springer-Verlag, Heidelberg, July 1991.

[18] V. Mehrmann. A step towards a unified treatment of continuous and discrete time control problems. *Linear Algebra Appl.*, to appear, 1996. *see also:* Preprint SPC 94_20, Fak. f. Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG.

[19] C.B. Moler and G.W. Stewart. An algorithm for generalized matrix eigenvalue problems. *SIAM J. Numer. Anal.*, 10:241–256, 1973.

[20] C.C. Paige and C.F. Van Loan. A Schur decomposition for Hamiltonian matrices. *Linear Algebra Appl.*, 14:11–32, 1981.

[21] R.V. Patel. On computing the eigenvalues of a symplectic pencil. *Linear Algebra Appl.*, 188/189:591–611, 1993. see also: Proc. CDC-31, Tuscon, AZ, 1992, pp. 1921–1926.

[22] G.W. Stewart. Determining the rank in the presence of errors. In M.S. Moonen, G.H. Golub, and B.L.R. de Moor, editors, *Linear Algebra for Large Scale and Real-Time Applications*, NATO ASI series, Dordrecht, 1993. Kluwer Academic.

[23] G.W. Stewart. Updating a rank revealing ULV decomposition. *SIAM J. Matrix Anal. Appl.*, 4:494–499, 1993.

[24] G.W. Stewart and J.-G. Sun. *Matrix Perturbation Theory.* Academic Press, New York, 1990.

[25] C.F. Van Loan. A symplectic method for approximating all the eigenvalues of a Hamiltonian matrix. *Linear Algebra Appl.*, 16:233–251, 1984.

[26] A. Varga. An LAPACK-based implementation of the periodic Schur decompsition, 1996. Preliminary version.

[27] J.H. Wilkinson. *The Algebraic Eigenvalue Problem.* Oxford University Press, Oxford, 1965.