A new method for computing the stable invariant subspace of a real Hamiltonian matrix or *Breaking Van Loan's curse?*

Peter Benner* Volker Mehrmann† Hongguo Xu‡

January 16, 1997

Dedicated to William B. Gragg on the occasion of his 60th birthday.

Abstract

A new backward stable, structure preserving method of complexity $\mathbf{O}(n^3)$ is presented for computing the stable invariant subspace of a real Hamiltonian matrix and the stabilizing solution of the continuous-time algebraic Riccati equation. The new method is based on the relationship between the invariant subspaces of the Hamiltonian matrix $\mathcal{H}$ and the extended matrix $\begin{bmatrix} 0 & \mathcal{H} \\ \mathcal{H} & 0 \end{bmatrix}$ and makes use of the symplectic URV-like decomposition that was recently introduced by the authors.

Keywords. Eigenvalue problem, Hamiltonian matrix, algebraic Riccati equation, sign function, invariant subspace.
AMS subject classification. 65F15, 93B40, 93B36, 93C60.

1 Introduction

It is a well accepted fact in numerical analysis that a numerical algorithm should reflect as many of the structural properties of the physical problem or the resulting mathematical model. For the solution of eigenvalue problems this means that use of the symmetry structures of the matrix or the spectrum is made. While for symmetric matrices this is relatively straight forward and well established [25], for other structures this is not the case. In the last ten years Bill Gragg and his co-workers (see, e.g., [3, 13, 14]) have made large contributions to the much more complicated orthogonal and unitary eigenvalue problems.

In this paper we now discuss another structured eigenvalue problem, the one for Hamiltonian matrices. It is a long-standing open problem [24] to compute the eigenvalues and the Lagrangian invariant subspaces (in particular the stable one) of Hamiltonian matrices via a

*Zentrum fuer Technomathematik, Fachbereich 3/Mathematik und Informatik, Postfach 330440 D-28334 Bremen, FRG. Supported by *Deutsche Forschungsgemeinschaft*, Research Grant Me 790/7-1.

†Fakultät für Mathematik, TU Chemnitz-Zwickau, D-09107 Chemnitz, FRG. Supported by *Deutsche Forschungsgemeinschaft*, Research Grant Me 790/7-1.

‡Department of Mathematics, Fudan University, Shanghai 200433, PR China. Current address: Fakultät für Mathematik, TU Chemnitz-Zwickau, D-09107 Chemnitz, FRG. This author was supported by *Alexander von Humboldt Foundation* and *Chinese National Natural Science Foundation.*

method that is of complexity $\mathbf{O}(n^3)$ and numerically strongly backward stable (in the sense of [6]), i.e., it is not only backward stable but the computed eigenvalues (subspaces) are the exact eigenvalues (subspaces) of a nearby Hamiltonian matrix. For completeness we recall the following definition.

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.*

a) 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* $\mathbf{H_{2n}}$. *We denote the subset of* $\mathbf{H}_{2n}$ *consisting of Hamiltonian matrices that have no eigenvalues on the imaginary axis by* $\mathbf{H^*_{2n}}$ *and by* $\mathbf{H^0_{2n}}$ *the set of Hamiltonian matrices, for which all the eigenvalues on the imaginary axis have even algebraic multiplicity. Matrices* $\mathcal{H} \in \mathbf{H_{2n}}$ *have the form* $\begin{bmatrix} F & G \\ H & -F^T \end{bmatrix}$, *where* $F, G, H \in \mathbf{R}^{n\times n}$, $G = G^T$, *and* $H = H^T$.

b) A matrix $\mathcal{S} \in \mathbf{R}^{2n\times 2n}$ *is called* **symplectic** *iff* $\mathcal{S}J\mathcal{S}^T = J$. *The Lie group of symplectic matrices in* $\mathbf{R}^{2n\times 2n}$ *is denoted by* $\mathbf{S}_{2n}$.

c) The group of orthogonal matrices in $\mathbf{R}^{n\times n}$ *is denoted by* $\mathbf{U_n}$.

d) A matrix $\mathcal{U} \in \mathbf{R}^{2n\times 2n}$ *is called* **orthogonal symplectic** *iff* $\mathcal{U} \in \mathbf{S}_{2n} \cap \mathbf{U}_{2n}$. *The Lie group of orthogonal symplectic matrices in* $\mathbf{R}^{2n\times 2n}$ *is denoted by* $\mathbf{US_{2n}}$. *Matrices* $\mathcal{U} \in \mathbf{US_{2n}}$ *have the form* $\mathcal{U} = \begin{bmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{bmatrix}$, *where* $U_1, U_2 \in \mathbf{R}^{n\times n}$.

The reason for the large interest in the solution of the Hamiltonian eigenvalue problem is its intimate relationship to the solution of the continuous-time algebraic Riccati equation

$$0 = F^T X + XF + H - XGX, \tag{1}$$

where F, G, H are the blocks in $\mathcal{H}$ and X is a real $n \times n$ symmetric matrix. It is well-known, that if X is symmetric and the columns of the matrix $\begin{bmatrix} I_n \\ -X \end{bmatrix}$ span an invariant subspace of $\mathcal{H}$ then X solves (1), e.g., [19, 24, 20, 23, 18].

Paige/Van Loan [24] showed that if $\mathcal{H} \in \mathbf{H^*_{2n}}$, then it has a Hamiltonian Schur-form, i.e. there exist a matrix $Q \in \mathbf{US_{2n}}$ such that

$$Q^T \mathcal{H} Q = \begin{bmatrix} T & N \\ 0 & -T^T \end{bmatrix}, \tag{2}$$

where T is quasi upper triangular and $N = N^T$. The first n columns of Q then span the desired Lagrangian subspace.

Lin and Ho [21] extended this result to the case that $\mathcal{H}$ has eigenvalues on the imaginary axis. In this case it is necessary but not sufficient for the existence of a Lagrangian subspace that the eigenvalues with zero real part have even algebraic multiplicity. But even if a Lagrangian subspace exists it is not always the case that it is spanned by the columns of a matrix of the form $\begin{bmatrix} I_n \\ -X \end{bmatrix}$, see [18] for details.

Example 1.2 If $\mathcal{H} = J \in \mathbf{US_4} \cap \mathbf{H_4}$ then there does not exist a matrix $Q \in \mathbf{US_4}$, such that

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

since $Q^T J Q = J$. But using a non-symplectic permutation matrix $\hat{Q} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ we obtain that $\hat{Q}^T J \hat{Q} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$ is in Hamiltonian Schur-form. Note that there exists no symmetric solution to (1).

Remark 1.3 Example 1.2 shows that Hamiltonian Schur-forms may exist, even if the transformation matrices are not symplectic. This does not contradict the result, that the only set of similarity transformations that leave $\mathbf{H_{2n}}$ invariant is $\mathbf{S_{2n}}$ (e.g. [7]), since in this case and also in the case that we study later in this paper, the Hamiltonian matrix has a special structure, in particular the diagonal blocks are 0. We will, therefore, in contrast to the existing literature require for a Hamiltonian Schur form only the existence of $U \in \mathbf{U_{2n}}$ such that

$$U^T \mathcal{H} U = \begin{bmatrix} T & N \\ 0 & -T^T \end{bmatrix}, \tag{3}$$

i.e., U need not be symplectic.

Unfortunately, the numerical computation of the Hamiltonian Schur form via a strongly backward stable $\mathbf{O}(n^3)$ method has been an open problem since its introduction. Many attempts have been made to solve this problem, see [8, 20, 23] and the references therein, but only in special cases a satisfactory solution has been obtained [9, 10]. Furthermore it has been shown in [1] that a modification of standard QR-like methods is in general hopeless, due to the missing reduction to a Hessenberg–like form. For this reason other methods like the multishift-method of [2] were developed that do not follow the direct line of a standard QR-like method. The multishift method is in principle a satisfactory solution, but unfortunately it sometimes has convergence problems, in particular for large n.

Recently the authors have proposed a method to compute the eigenvalues (but not the invariant subspaces) of Hamiltonian matrices using a new approach via non-similarity transformations. This new method is based on the following symplectic URV-like decomposition:

Lemma 1.4 (Symplectic URV Decomposition) *Let $\mathcal{H} \in \mathbf{H_{2n}}$, then there exist $U_1, U_2 \in \mathbf{US_{2n}}$ such that*

$$\mathcal{H} = U_2 \begin{bmatrix} H_t & H_r \\ 0 & -H_b^T \end{bmatrix} U_1^T, \tag{4}$$

where $H_t, H_r, H_b \in \mathbf{R}^{n \times n}$, H_t is upper triangular and H_b is quasi upper triangular (diagonal blocks of sizes 1×1 or 2×2). Moreover,

$$\mathcal{H} = J \mathcal{H}^T J = U_1 \begin{bmatrix} H_b & H_r^T \\ 0 & -H_t^T \end{bmatrix} U_2^T \tag{5}$$

and the positive and negative square roots of the eigenvalues of $H_t H_b$ are the eigenvalues of $\mathcal{H}$.

Proof. See [5]. □

Using this URV-like decomposition the authors presented in [5] a new method to compute the eigenvalues of a Hamiltonian matrix. This is a generalization of the square-reduced method of Van Loan [28] but in contrast to that method it achieves the full possible accuracy. There have also been several attempts to build a method for the computation of invariant subspaces on the square reduced approach [30, 31], but so far none of these approaches lead to a numerically stable procedure.

In this paper we now present a new idea that is based on the new eigenvalue method of [5] and yields a new method that is not only backward stable, and of complexity $\mathbf{O}(n^3)$, but also structure preserving.

The key idea for this new method is to employ the relationship between the eigenvalues and invariant subspaces of $\mathcal{H}$ and the extended matrix $\begin{bmatrix} 0 & \mathcal{H} \\ \mathcal{H} & 0 \end{bmatrix}$. In principle it can be applied also to arbitrary matrices and it gives a new way to determine the sign function of A or the positive square root of A^2, [26, 16], but for general matrices it will not be efficient. For Hamiltonian matrices, however, the new idea can significantly exploit the structure to be efficient.

The paper is organized as follows: In Section 2 we develop the general theoretical background for the new algorithm and in Section 3 we then specialize these results to the Hamiltonian case and describe the new procedure. An error analysis is given in Section 4 and numerical examples are presented in Section 5. Some algorithmic details for the new procedure are given in the appendix.

We use the following notation: The spectrum (including multiple eigenvalues) of a matrix $A \in \mathbf{R}^{n\times n}$ is denoted by $\lambda(A)$. The subsets of $\lambda(A)$ of eigenvalues with positive, zero, and negative real parts, respectively, are denoted by $\lambda_+(A)$, $\lambda_0(A)$, and $\lambda_-(A)$, respectively. The associated invariant subspaces of A corresponding to these subsets of eigenvalues are denoted by $\mathrm{Inv}_+(A)$, $\mathrm{Inv}_0(A)$, $\mathrm{Inv}_-(A)$, respectively. Finally $\|\cdot\|$ refers to the spectral norm.

2 Theoretical Background

In this section we give the theoretical background for our new method. This approach can also be applied to general matrices, so we present it in general and then show how it specializes for Hamiltonian matrices in the next section. Let $A \in \mathbf{R}^{n\times n}$ and consider the eigenstructure of the extended matrix

$$B = \begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix}. \tag{6}$$

Let $\hat{I} = \frac{\sqrt{2}}{2}\begin{bmatrix} I_n & -I_n \\ I_n & I_n \end{bmatrix} \in \mathbf{US_{2n}}$, then

$$\hat{I}^T B \hat{I} = \begin{bmatrix} A & 0 \\ 0 & -A \end{bmatrix}. \tag{7}$$

This implies the following relationship between the spectra of A and B.

$$
\begin{aligned}
\lambda(B) &= \lambda(A) \cup \lambda(-A), \\
\lambda_0(B) &= \lambda_0(A) \cup \lambda_0(A), \\
\lambda_+(B) &= \lambda_+(A) \cup \lambda_+(-A) \;=\; \lambda_+(A) \cup (-\lambda_-(A)), \\
\lambda_-(B) &= \lambda_-(A) \cup \lambda_-(-A) \;=\; (-\lambda_+(A)) \cup \lambda_-(A) \;=\; -\lambda_+(B).
\end{aligned} \tag{8}
$$

(Note that in the spectra we count eigenvalues with their algebraic multiplicities.) We obtain the following relations for the invariant subspaces of A and B.

Theorem 2.1 *Let $A \in \mathbf{R}^{n\times n}$ and $B \in \mathbf{R}^{2n\times 2n}$ be related as in (6) and let $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \in \mathbf{R}^{2n\times n}$, $Q_1, Q_2 \in \mathbf{R}^{n\times n}$, have orthonormal columns, such that*

$$
B \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R, \tag{9}
$$

where

$$
\lambda_+(B) \subseteq \lambda(R) \subseteq \lambda_+(B) \cup \lambda_0(B). \tag{10}
$$

Then

$$
\mathrm{range}\{Q_1 + Q_2\} = \mathrm{Inv}_+(A) + \mathcal{N}_1, \quad \textit{where} \quad \mathcal{N}_1 \subseteq \mathrm{Inv}_0(A), \tag{11}
$$

$$
\mathrm{range}\{Q_1 - Q_2\} = \mathrm{Inv}_-(A) + \mathcal{N}_2, \quad \textit{where} \quad \mathcal{N}_2 \subseteq \mathrm{Inv}_0(A). \tag{12}
$$

Moreover, if we partition R as

$$
R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}, \; \textit{where } \lambda(R_{11}) = \lambda_+(B), \tag{13}
$$

and, accordingly, $Q_1 = \begin{bmatrix} Q_{11} & Q_{12} \end{bmatrix}$, $Q_2 = \begin{bmatrix} Q_{21} & Q_{22} \end{bmatrix}$, then

$$
B \begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix} = \begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix} R_{11}, \tag{14}
$$

and there exists an orthogonal matrix Z such that

$$
\frac{\sqrt{2}}{2}(Q_{11} + Q_{21}) = \begin{bmatrix} 0 & P_+ \end{bmatrix} Z, \qquad \frac{\sqrt{2}}{2}(Q_{11} - Q_{21}) = \begin{bmatrix} P_- & 0 \end{bmatrix} Z, \tag{15}
$$

where P_+, P_- are orthogonal bases of $\mathrm{Inv}_+(A)$, $\mathrm{Inv}_-(A)$, *respectively.*

Proof. Identity (9) implies that $AQ_2 = Q_1 R$ and $AQ_1 = Q_2$R. Hence

$$
A(Q_1 + Q_2) = (Q_1 + Q_2)R, \qquad A(Q_1 - Q_2) = (Q_1 - Q_2)(-R).
$$

By (10) we have

$$
\mathrm{range}\{Q_1 + Q_2\} \subseteq \mathrm{Inv}_+(A) + \mathrm{Inv}_0(A), \tag{16}
$$

$$
\mathrm{range}\{Q_1 - Q_2\} \subseteq \mathrm{Inv}_-(A) + \mathrm{Inv}_0(A). \tag{17}
$$

Since $\lambda_+(B) \subseteq \lambda(R)$, we may assume w.l.o.g. that R is in the form (13) and that we have (14). With the same argumentation used to derive (16) and (17) we get

$$\operatorname{range}\{Q_{11}+Q_{21}\} \subseteq \operatorname{Inv}_+(A), \qquad \operatorname{range}\{Q_{11}-Q_{21}\} \subseteq \operatorname{Inv}_-(A).$$

If $R_{11} \in \mathbf{R}^{p\times p}$, then $\dim \operatorname{Inv}_+(A) + \dim \operatorname{Inv}_-(A) = p$. Hence,

$$\operatorname{rank}(Q_{11}+Q_{21}) + \operatorname{rank}(Q_{11}-Q_{21}) \leq p.$$

On the other hand, with

$$\frac{\sqrt{2}}{2}\begin{bmatrix} Q_{11}+Q_{21} \\ Q_{11}-Q_{21} \end{bmatrix} = \hat{I}\begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix}, \tag{18}$$

and using that $\hat{I}$ and $\begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix}$ are orthogonal, we obtain that

$$\operatorname{rank}(Q_{11}+Q_{21}) + \operatorname{rank}(Q_{11}-Q_{21}) \geq \operatorname{rank}\begin{bmatrix} Q_{11}+Q_{21} \\ Q_{11}-Q_{21} \end{bmatrix} = p.$$

Hence, $\operatorname{rank}(Q_{11}+Q_{21}) + \operatorname{rank}(Q_{11}-Q_{21}) = p$ and since it is clear that $\operatorname{range}\{Q_{11}+Q_{21}\} \cap \operatorname{range}\{Q_{11}-Q_{21}\} = \{0\}$, it follows that

$$\operatorname{range}\{Q_{11}+Q_{21}\} = \operatorname{Inv}_+(A), \qquad \operatorname{range}\{Q_{11}-Q_{21}\} = \operatorname{Inv}_-(A). \tag{19}$$

Combining this with (16), (17) we obtain (11) and (12).

Now let $Z \in \mathbf{U_p}$ such that

$$\frac{\sqrt{2}}{2}(Q_{11}-Q_{21})Z^T = \begin{bmatrix} P_- & 0 \end{bmatrix},$$

and P_- has full column rank, i.e., the columns of P_- form a basis of $\operatorname{Inv}_-(A)$. Define

$$C := \frac{\sqrt{2}}{2}\begin{bmatrix} Q_{11}+Q_{21} \\ Q_{11}-Q_{21} \end{bmatrix} Z^T =: \begin{bmatrix} P_{11} & P_+ \\ P_- & 0 \end{bmatrix},$$

then from (18), C is orthonormal, so P_+ must be orthonormal, i.e., $P_+^T P_+ = I$. It is obvious that $\operatorname{rank} P_+ = p - \operatorname{rank} P_- = p - \dim \operatorname{Inv}_-(A) = \dim \operatorname{Inv}_+(A)$. Thus, the columns of P_+ form an orthogonal basis of $\operatorname{Inv}_+(A)$. With (19) we get

$$\operatorname{Inv}_+(A) \;=\; \operatorname{range}\{P_+\} \;=\; \operatorname{range}\{\begin{bmatrix} P_{11} & P_+ \end{bmatrix}\}.$$

Thus, there must exist a matrix $\hat{Z}$, such that $P_{11} = P_+\hat{Z}$. Again, since C is orthonormal, we have $P_{11}^T P_+ = 0$, which implies $0 = \hat{Z}^T P_+^T P_+ = \hat{Z}^T$, i.e., $P_{11} = 0$. Therefore P_- is also orthonormal and we have (15). $\square$

Remark 2.2

a) If in Theorem 2.1, the assumption of $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ having orthonormal columns is relaxed to assuming full column rank, then we still obtain results analogous to (12)–(14).

b) The number of columns of $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ (or the size of R) can be chosen in the interval $[p, 2n-p]$, where $p = \dim \mathrm{Inv}_+(A) + \dim \mathrm{Inv}_-(A)$, i.e., the spectrum of R may contain any number of eigenvalues from $\lambda_0(B)$ as long as these admit a real invariant subspace of B.

c) If we just assume that $\lambda_-(R) = \emptyset$ instead of (10), we only obtain (16) and (17). If $\lambda(R) \subseteq \lambda_+(B)$, then $\mathrm{range}\{Q_1 + Q_2\} \subseteq \mathrm{Inv}_+(A)$ and $\mathrm{range}\{Q_1 - Q_2\} \subseteq \mathrm{Inv}_-(A)$.

If A has no purely imaginary eigenvalues then we have the following corollary as a direct consequence of Theorem 2.1.

Corollary 2.3 *Under the hypotheses of Theorem 2.1 and assuming further that* $\lambda_0(A) = \emptyset$, *there exists* $Z \in \mathbf{U_n}$ *such that*

$$\frac{\sqrt{2}}{2}(Q_1 + Q_2) = \begin{bmatrix} 0 & P_+ \end{bmatrix} Z, \qquad \frac{\sqrt{2}}{2}(Q_1 - Q_2) = \begin{bmatrix} P_- & 0 \end{bmatrix} Z, \tag{20}$$

where P_+, P_- *are orthogonal bases of* $\mathrm{Inv}_+(A)$ *and* $\mathrm{Inv}_-(A)$, *respectively.*

The above results give a direct relationship between a matrix, its sign function, and the square root of its square. To see this, assume that $\lambda_0(A) = \emptyset$. Then there exists a nonsingular matrix X such that

$$A = X \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix} X^{-1},$$

where T_1 is a $k \times k$ matrix, $\lambda(T_1) = \lambda_+(A)$ and $\lambda(T_2) = \lambda_-(A)$. The matrix

$$X \begin{bmatrix} I_k & 0 \\ 0 & -I_{n-k} \end{bmatrix} X^{-1}$$

is the *sign function matrix* of A, denoted by $\mathrm{Sign}(A)$, (e.g. [26, 16]), and the matrix $X \begin{bmatrix} T_1 & 0 \\ 0 & -T_2 \end{bmatrix} X^{-1}$ is the *positive square root* of A^2, denoted by $\mathrm{Sqrt}(A^2)$, see e.g., [17].

The matrices A, $\mathrm{Sign}(A)$, $\mathrm{Sqrt}(A^2)$ commute, and

$$\mathrm{Sign}(A)^2 = I_n, \tag{21}$$

$$A\,\mathrm{Sign}(A) = \mathrm{Sqrt}(A^2), \qquad A = \mathrm{Sign}(A)\,\mathrm{Sqrt}(A^2), \tag{22}$$

see [16]. Also we have [26, 30, 31]

$$\mathrm{range}\{\mathrm{Sign}(A) + I_n\} = \mathrm{range}\{A + \mathrm{Sqrt}(A^2)\} = \mathrm{Inv}_+(A), \tag{23}$$

$$\mathrm{range}\{\mathrm{Sign}(A) - I_n\} = \mathrm{range}\{A - \mathrm{Sqrt}(A^2)\} = \mathrm{Inv}_-(A). \tag{24}$$

Theorem 2.4 *Let* A, B, Q_1, Q_2, R *be as in Theorem 2.1. If* $\lambda_0(A) = \emptyset$, *then* Q_1 *and* Q_2 *are nonsingular, and*

$$\begin{array}{rcccl} \mathrm{Sign}(A) & = & Q_1 Q_2^{-1} & = & Q_2 Q_1^{-1}, \\ \mathrm{Sqrt}(A^2) & = & Q_1 R Q_1^{-1} & = & Q_2 R Q_2^{-1}. \end{array} \tag{25}$$

Proof. We can rewrite the equations of (22) as

$$B \begin{bmatrix} I_n \\ \mathrm{Sign}(A) \end{bmatrix} = \begin{bmatrix} I_n \\ \mathrm{Sign}(A) \end{bmatrix} \mathrm{Sqrt}(A^2).$$

Then

$$\lambda(\mathrm{Sqrt}(A^2)) = \lambda_+(B) = \lambda(R),$$

and hence both $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$, $\begin{bmatrix} I_n \\ \mathrm{Sign}(A) \end{bmatrix}$ span $\mathrm{Inv}_+(B)$.

Since $\mathrm{Inv}_+(B)$ is unique, there must be a nonsingular matrix Z such that

$$\begin{bmatrix} I_n \\ \mathrm{Sign}(A) \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} Z, \quad \text{i.e.,} \quad Q_1 Z = I_n,\ Q_2 Z = \mathrm{Sign}(A).$$

By (21), $\mathrm{Sign}(A)$ is nonsingular. Thus Q_1 and Q_2 are nonsingular and $\mathrm{Sign}(A) = Q_2 Q_1^{-1}$. Using $\mathrm{Sign}(A) = \mathrm{Sign}(A)^{-1}$ we also get $\mathrm{Sign}(A) = Q_1 Q_2^{-1}$.

From (9) we obtain $AQ_2 = Q_1 R$ and $AQ_1 = Q_2 R$ and applying (22)

$$\begin{aligned} \mathrm{Sqrt}(A^2) = A\,\mathrm{Sign}(A) &= AQ_2Q_1^{-1} = Q_1 R Q_1^{-1} \\ &= AQ_1Q_2^{-1} = Q_2 R Q_2^{-1}. \end{aligned} \qquad \square$$

Remark 2.5 If $\lambda_0(A) \neq \emptyset$, then $\mathrm{Sign}(A)$ and $\mathrm{Sqrt}(A^2)$ are not defined, but Q_1, Q_2 and R always exist. These matrices can be considered as generalizations of $\mathrm{Sign}(A)$ and $\mathrm{Sqrt}(A^2)$. Note further that the results in Theorem 2.1 generalize the formulas (23) and (24).

The results in this section indicate how to obtain a numerical method for the computation of the invariant subspaces $\mathrm{Inv}_+(A)$ and $\mathrm{Inv}_-(A)$ via the Schur form of B. In general, this is not a suitable method, because we can easily compute invariant subspaces by first forming the Schur form of A and then reordering the eigenvalues. However, when this approach is applied to real Hamiltonian matrices, then it turns out to be very useful as we will show in the following sections.

3 Application to Hamiltonian Matrices

In this section we discuss how the general ideas of the previous section specialize to the case of Hamiltonian matrices. We will in general assume that $\mathcal{H} \in \mathbf{H}^*_{\mathbf{2n}}$ and we will point out where the results hold in a more general situation like $\mathcal{H} \in \mathbf{H}^{\mathbf{0}}_{\mathbf{2n}}$. We consider the block matrix

$$\mathcal{B} = \begin{bmatrix} 0 & \mathcal{H} \\ \mathcal{H} & 0 \end{bmatrix}. \tag{26}$$

Observe that $\tilde{\mathcal{B}} := \mathrm{diag}(I_{2n}, J^{-1})\mathcal{B}\,\mathrm{diag}(I_{2n}, J) \in \mathbf{H}^*_{\mathbf{4n}}$, since $\mathcal{H} \in \mathbf{H}^*_{\mathbf{2n}}$ implies that $\mathcal{H}J$ and $J^{-1}\mathcal{H} = J^T\mathcal{H}$ are symmetric and by (8) it follows that $\lambda_0(\tilde{\mathcal{B}}) = \emptyset$.

We have the following main result which we prove constructively.

Theorem 3.1 *Let $\mathcal{H} \in \mathbf{H^0_{2n}}$ and $\mathcal{B}$ as in (26). Then there exists $\mathcal{U} \in \mathbf{U_{4n}}$ such that*

$$\mathcal{U}^T \mathcal{B} \mathcal{U} = \begin{bmatrix} R & D \\ 0 & -R^T \end{bmatrix} =: \mathcal{R}, \tag{27}$$

is in Hamiltonian Schur form and $\lambda_-(R) = \emptyset$. Furthermore, if $\mathcal{H} \in \mathbf{H^*_{2n}}$, then $\mathcal{R}$ has only eigenvalues with positive real part. Moreover, $\mathcal{U} = \hat{\mathcal{U}}\mathcal{P}\tilde{\mathcal{U}}$ with $\tilde{\mathcal{U}} \in \mathbf{US}_{4n}$,

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

and $\hat{\mathcal{U}} = \mathrm{diag}(U_1, U_2)$, where $U_1, U_2 \in \mathbf{US}_{2n}$.

Proof. We will make use of the symplectic URV decompositions of $\mathcal{H}$. By Lemma 1.4 there exist $U_1, U_2 \in \mathbf{US_{2n}}$, such that

$$\mathcal{H} = U_2 \begin{bmatrix} H_t & H_r \\ 0 & -H_b^T \end{bmatrix} U_1^T, \tag{28}$$

$$\mathcal{H} = U_1 \begin{bmatrix} H_b & H_r^T \\ 0 & -H_t^T \end{bmatrix} U_2^T, \tag{29}$$

where H_t is upper triangular and H_b is quasi-upper triangular. Taking $\hat{\mathcal{U}} := \mathrm{diag}(U_1, U_2)$, we have

$$\mathcal{B}_1 := \hat{\mathcal{U}}^T \mathcal{B} \hat{\mathcal{U}} = \left[\begin{array}{cc|cc} 0 & 0 & H_b & H_r^T \\ 0 & 0 & 0 & -H_t^T \\ \hline H_t & H_r & 0 & 0 \\ 0 & -H_b^T & 0 & 0 \end{array}\right]. \tag{30}$$

Using the block form of $\mathcal{P}$,

$$\mathcal{B}_2 := \mathcal{P}^T \mathcal{B}_1 \mathcal{P} = \left[\begin{array}{cc|cc} 0 & H_b & 0 & H_r^T \\ H_t & 0 & H_r & 0 \\ \hline 0 & 0 & 0 & -H_t^T \\ 0 & 0 & -H_b^T & 0 \end{array}\right]$$

is Hamiltonian and block upper triangular. Let $U_3 = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix} \in \mathbf{U_{2n}}$ be such that

$$U_3^T \begin{bmatrix} 0 & H_b \\ H_t & 0 \end{bmatrix} U_3 =: \begin{bmatrix} \Sigma & \Gamma \\ 0 & -\Delta \end{bmatrix}, \tag{31}$$

is in real Schur form with Σ, $\Delta \in \mathbf{R}^{n \times n}$ quasi upper triangular and

$$\lambda(\Sigma) = \lambda(\Delta),\ \lambda_-(\Sigma) = \emptyset. \tag{32}$$

Then

$$\mathcal{B}_3 := \begin{bmatrix} U_3 & 0 \\ 0 & U_3 \end{bmatrix}^T \mathcal{B}_2 \begin{bmatrix} U_3 & 0 \\ 0 & U_3 \end{bmatrix} = \left[\begin{array}{cc|cc} \Sigma & \Gamma & \Pi_1 & \Pi_2 \\ 0 & -\Delta & \Pi_2^T & \Pi_3 \\ \hline 0 & 0 & -\Sigma^T & 0 \\ 0 & 0 & -\Gamma^T & \Delta^T \end{array}\right]. \tag{33}$$

Note that $\mathcal{B}_3$ is already in Hamiltonian Schur form. The order of the eigenvalues on the block diagonal may, however, be not as we require. But using the reordering procedure of Byers [9, 10], there exists an orthogonal symplectic matrix $\mathcal{V} := \left[\begin{array}{cc|cc} I_n & 0 & 0 & 0 \\ 0 & V_1 & 0 & V_2 \\ \hline 0 & 0 & I_n & 0 \\ 0 & -V_2 & 0 & V_1 \end{array}\right] \in \mathbf{US_{4n}}$ such that

$$\mathcal{R} := \mathcal{V}^T \mathcal{B}_3 \mathcal{V} = \left[\begin{array}{cc|cc} \Sigma & \tilde{\Gamma} & \Pi_1 & \tilde{\Pi}_2 \\ 0 & \tilde{\Delta} & \tilde{\Pi}_2^T & \tilde{\Pi}_3 \\ \hline 0 & 0 & -\Sigma^T & 0 \\ 0 & 0 & -\tilde{\Gamma}^T & -\tilde{\Delta}^T \end{array}\right]. \tag{34}$$

is in Hamiltonian Schur form with the required eigenvalue reordering and $\tilde{\mathcal{U}} := \mathrm{diag}(U_3, U_3)\mathcal{V} \in \mathbf{US}_{4n}$. $\square$

Remark 3.2 The transformation matrix U_3 in the proof of Theorem 3.1 can be obtained in an efficient way by exploiting the structure of $\begin{bmatrix} 0 & H_b \\ H_t & 0 \end{bmatrix}$, recalling that H_b is already quasi-upper triangular and H_t is upper triangular. For details of this reduction see the appendix.

If we partition $\mathcal{U} := \begin{bmatrix} \mathcal{U}_{11} & \mathcal{U}_{12} \\ \mathcal{U}_{21} & \mathcal{U}_{22} \end{bmatrix}$, $\mathcal{U}_{ij} \in \mathbf{R}^{2n\times 2n}$, then using the structures of the matrices $\hat{\mathcal{U}}$, $\mathcal{P}$, U_3 and $\mathcal{V}$ we obtain

$$\mathcal{U}_{11} = U_2 \begin{bmatrix} U_{11} & U_{12}V_1 \\ 0 & -U_{12}V_2 \end{bmatrix}, \qquad \mathcal{U}_{21} = U_1 \begin{bmatrix} U_{21} & U_{22}V_1 \\ 0 & -U_{22}V_2 \end{bmatrix}. \tag{35}$$

By Theorem 2.1 we have

$$\mathrm{range}\{\mathcal{U}_{11} - \mathcal{U}_{21}\} = \mathrm{Inv}_-(\mathcal{H}) + \mathcal{N}_1, \qquad \mathrm{range}\{\mathcal{U}_{11} + \mathcal{U}_{21}\} = \mathrm{Inv}_+(\mathcal{H}) + \mathcal{N}_2, \tag{36}$$

where $\mathcal{N}_1$, $\mathcal{N}_2 \subset \mathrm{Inv}_0(\mathcal{H})$. Clearly, if $\mathcal{H} \in \mathbf{H_{2n}^*}$ then, since $\mathrm{Inv}_0(\mathcal{H}) = \emptyset$, we have computed the required subspace.

The construction in the proof of Theorem 3.1 leads to the following algorithm for computing the desired (stable) invariant subspace of a Hamiltonian matrix $\mathcal{H} \in \mathbf{H_{2n}^*}$. The computation of the unstable invariant subspace can be done simultaneously.

Algorithm 1 *This algorithm computes the Lagrangian invariant subspace of a Hamiltonian matrix $\mathcal{H} \in \mathbf{H_{2n}^*}$, corresponding to the eigenvalues in the left half plane.*

Input: *A Hamiltonian matrix $\mathcal{H} \in \mathbf{H_{2n}^*}$.*

Output: $Y \in \mathbf{R}^{2n\times n}$, *with* $Y^TY = I_n$, $\mathrm{range}\{Y\} = \mathrm{Inv}_-(\mathcal{H})$.

Step 1 *Apply Algorithm 2 of [5] to $\mathcal{H}$ and compute the symplectic URV decomposition,*

$$\mathcal{H} := U_2 \begin{bmatrix} H_t & H_r \\ O & -H_b^T \end{bmatrix} U_1^T, \qquad U_1, U_2 \in \mathbf{US}_{2n}.$$

Step 2 *Determine U_3, Δ as in (31). Compute Π_3 as in (33).*

Step 3 *Compute $\mathcal{V}$ from the orthogonal symplectic reordering scheme of Byers [10].*

Step 4 *Form $\mathcal{U}_{11}$, $\mathcal{U}_{21}$ as in (35). Set $\hat{Y} := \frac{\sqrt{2}}{2}(\mathcal{U}_{11} - \mathcal{U}_{21})$. Compute Y, an orthogonal basis of* $\mathrm{range}\{\hat{Y}\}$*, using any numerically stable orthogonalization scheme, for example a rank-revealing QR-decomposition; see, e.g., [11].*

End

Remark 3.3 In the last step of Algorithm 1, a QR factorization is usually sufficient to determine the required invariant subspace because of (20). But in general it is more reliable to use a rank-revealing QR-decomposition, see e.g. [11].

We have estimated the computational cost for this algorithm under the following assumptions. We assume that the periodic QR-iteration needs an average of two iterations per eigenvalue, that the diagonal blocks in H_b are all 2×2, that we used a rank-revealing QR decomposition in Step 4 and the method described in the appendix in Step 2. The flop counts for the four steps are given in Table 1.

Step	1	2	3	4	total
flops	$103\ n^3$	$9\ n^3$	$9\ n^3$	$42\ n^3$	$163\ n^3$

Table 1: Flop counts for Algorithm 1

These numbers compare with $203n^3$ flops for the computation of the same invariant subspace via the standard QR-algorithm as suggested in [19].

The storage requirement for this algorithm is about $9n^2$, a little more than for the standard QR algorithm.

Remark 3.4 Up to now we have discussed only the computation of the stable invariant subspace of the Hamiltonian matrix and not the solution of algebraic Riccati equation (1), since the invariant subspace computation is more general and can also be used in other applications. Clearly we can obtain the stabilizing solution of the Riccati equation from the invariant subspace but it is also possible to get it directly from $\hat{Y}$. As both, $range(\hat{Y})$ and $range\left(\begin{bmatrix} I \\ -X \end{bmatrix}\right)$ form a basis of $Inv_-(\mathcal{H})$ and moreover, $Inv_-(\mathcal{H})$ is isotropic with respect to the inner product defined by $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$ (see, e.g., [18]), we have

$$\begin{bmatrix} I \\ -X \end{bmatrix}^T JY = \begin{bmatrix} X & I_n \end{bmatrix} \hat{Y} = 0.$$

Let $\hat{Y} = \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \end{bmatrix}$, $\hat{Y}_1, \hat{Y}_2 \in \mathbf{R}^{n \times 2n}$, then $X\hat{Y}_1 = -\hat{Y}_2$. The solution X can thus be computed directly by solving this overdetermined, consistent set of linear equations. In this case it is not necessary to explicitly form an orthogonal basis for $range(\hat{Y})$ as in Step 4 of Algorithm 1.

Remark 3.5 By Remark 2.2 c), as long as $\lambda(R) \subseteq \lambda_+(B)$, range$\{Q_1 - Q_2\} \subseteq \mathrm{Inv}_-(A)$ regardless of the size of R. So in Algorithm 1 we can easily check whether

$$\mathrm{range}\{U_2 \begin{bmatrix} U_{11} \\ 0 \end{bmatrix} - U_1 \begin{bmatrix} U_{21} \\ 0 \end{bmatrix}\} = \mathrm{Inv}_-(\mathcal{H})$$

after we have finished Step 2. If the subspace is satisfactory, then we may stop the algorithm after Step 2, otherwise we continue the process. In general, however, it may happen that $\mathrm{rank}(Q_1 - Q_2) < \dim \mathrm{Inv}_-(A)$, i.e., some basis vectors of the invariant subspace are missing, or the computed bases are not accurate. We will demonstrate this phenomenon in some examples in Section 5. If we stop after Step 2 then the computational cost reduces to $118n^3$ flops and the storage requirement reduces to $8n^2$.

Remark 3.6 Algorithm 1 can also be applied to matrices with eigenvalues on the imaginary axis. But in this case it is not clear which invariant subspace we wish to compute, i.e., which of the eigenvectors and principal vectors corresponding to purely imaginary eigenvalues should be contained in the desired subspace. In this case it is also sometimes difficult to decide in finite precision arithmetic whether a Lagrangian subspace exists, because this depends on the partial multiplicities of the eigenvalues, see [18, 21]. These questions are currently under investigation.

4 Error Analysis

In this section we present an error analysis for Algorithm 1 applied to matrices in $\mathbf{H^*_{2n}}$. We show that the method computes the Hamiltonian Schur form of a (typically) non-Hamiltonian matrix close to $\tilde{\mathcal{B}}$. This is not quite what we would like to have. It would be better if the matrix for which we obtain the Hamiltonian Schur form is Hamiltonian itself and it would be ideal to compute the Hamiltonian Schur form of $\mathcal{H}$ directly, without having to use $\mathcal{B}$ or $\tilde{\mathcal{B}}$. How to get these better methods is still an open problem.

In the following we use $\mathrm{Sep}(A, B) := \min_{X \neq 0} \frac{\|AX - XB\|}{\|X\|}$, where $\|\,.\,\|$ is the spectral norm, and by ϵ we denote the machine precision. We first introduce several lemmata.

Lemma 4.1 *Suppose that $\mathcal{H} \in \mathbf{H}^*_{2n}$ has the Hamiltonian Schur form*

$$Q^T \mathcal{H} Q = \begin{bmatrix} T & N \\ 0 & -T^T \end{bmatrix}$$

with $\lambda(T) = \lambda_-(\mathcal{H})$. Let $P = \begin{bmatrix} P_1 & P_2 \\ -P_2 & P_1 \end{bmatrix} \in \mathbf{US_{2n}}$ be such that

$$P^T \begin{bmatrix} -T^T & 0 \\ N & T \end{bmatrix} P = \begin{bmatrix} -\hat{T}^T & \hat{N} \\ 0 & \hat{T} \end{bmatrix}$$

with $\lambda(\hat{T}) = \lambda(T) = \lambda_-(\mathcal{H})$. Let

$$\mathcal{Q} := \frac{\sqrt{2}}{2} \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix} \left[\begin{array}{cc|cc} I_n & 0 & I_n & 0 \\ 0 & I_n & 0 & -I_n \\ \hline -I_n & 0 & I_n & 0 \\ 0 & I_n & 0 & I_n \end{array}\right] \left[\begin{array}{cc|cc} I_n & 0 & 0 & 0 \\ 0 & P_1 & 0 & P_2 \\ \hline 0 & -P_2 & 0 & P_1 \\ 0 & 0 & I_n & 0 \end{array}\right], \tag{37}$$

then

$$\mathcal{Q}^T\mathcal{B}\mathcal{Q} = \left[\begin{array}{cc|cc} -T & 0 & N & 0 \\ 0 & -\hat{T}^T & 0 & \hat{N} \\ \hline 0 & 0 & T^T & 0 \\ 0 & 0 & 0 & \hat{T} \end{array}\right] =: \left[\begin{array}{cc} M & S \\ 0 & -M^T \end{array}\right] \in \mathbf{H}^*_{4n}. \tag{38}$$

Proof. The proof follows by direct calculation. □

Lemma 4.2 *Let M be as in (38) then*

$$\delta := \mathrm{Sep}(M^T, -M) = \min\{\mathrm{Sep}(T^T, -T), \mathrm{Sep}(\hat{T}, -\hat{T}^T)\}. \tag{39}$$

Proof. Since $\lambda(M) = \lambda_+(M)$, applying the results in [15], we have $\mathrm{Sep}(M^T, -M) = 1/\|X\|$, where X is the solution of the Lyapunov equation $M^TX + XM = I_{2n}$. Since $M = \mathrm{diag}(-T, -\hat{T}^T)$ and $\lambda(T) = \lambda(\hat{T}) = \lambda_-(\mathcal{H})$, it follows that $X = \mathrm{diag}(X_1, X_2)$, where X_j, $j = 1, 2$, are the solutions of the Lyapunov equations $T^TX_1 + X_1T = -I_n$, $\hat{T}X_2 + X_2\hat{T}^T = -I_n$. Then, again from [15], we have $\mathrm{Sep}(T^T, -T) = 1/\|X_1\|$ and $\mathrm{Sep}(\hat{T}, -\hat{T}^T) = 1/\|X_2\|$. Hence, $\|X\| = \max\{\|X_1\|, \|X_2\|\}$ implies (39). □

Our next result gives a structured forward error analysis for the computation of the Hamiltonian Schur form of $\mathcal{B}$.

Lemma 4.3 *If $\mathcal{R}$, $\mathcal{U}$ are the computed factors in the Hamiltonian Schur form (27) of $\mathcal{B}$ determined by Algorithm 1, then*

$$\mathcal{U}^T\mathcal{B}\mathcal{U} = \mathcal{R} + \mathcal{E}, \tag{40}$$

where

$$\mathcal{E} \in \mathbf{H}_{4n}, \qquad \|\mathcal{E}\| \leq c\epsilon\|\mathcal{H}\|, \tag{41}$$

and c is some constant.

Proof. Using standard backward error analysis [29], since $U_1, U_2 \in \mathbf{U_n}$, there exists

$$F = \left[\begin{array}{cc} F_{11} & F_{12} \\ F_{21} & F_{22} \end{array}\right] \in \mathbf{R}^{2n\times 2n}, \qquad \|F\| \leq c_1\epsilon\|\mathcal{H}\|,$$

such that (rewritten in a forward way)

$$U_2^T\mathcal{H}U_1 = \left[\begin{array}{cc} H_t & H_r \\ 0 & -H_b^T \end{array}\right] + F, \qquad U_1^T\mathcal{H}U_2 = \left[\begin{array}{cc} H_b & H_r^T \\ 0 & -H_t^T \end{array}\right] + JF^TJ.$$

So with $\hat{\mathcal{U}}$, $\mathcal{P}$ as in Theorem 3.1,

$$\mathcal{P}^T\hat{\mathcal{U}}^T\mathcal{B}\hat{\mathcal{U}}\mathcal{P} = \mathcal{P}^T(\mathcal{B}_1 + \left[\begin{array}{cc} 0 & JF^TJ \\ F & 0 \end{array}\right])\mathcal{P} =: \mathcal{B}_2 + \mathcal{E}_1,$$

where $\mathcal{B}_2 \in \mathbf{H}^0_{4n}$ and

$$\mathcal{E}_1 = \left[\begin{array}{cc|cc} 0 & -F_{22}^T & 0 & F_{12}^T \\ F_{11} & 0 & F_{12} & 0 \\ \hline 0 & F_{21}^T & 0 & -F_{11}^T \\ F_{21} & 0 & F_{22} & 0 \end{array}\right] \in \mathbf{H}_{4n}$$

satisfies $\|\mathcal{E}_1\| = \|F\| \leq c_1\epsilon\|\mathcal{H}\|$. Note that the matrix F in general is not Hamiltonian and note further that we cannot guarantee that $\mathcal{B}_2 \in \mathbf{H}^*_{4n}$, since perturbations may have moved eigenvalues on the imaginary axis.

Steps 2 and 3 of Algorithm 1 only use $4n\times 4n$ orthogonal symplectic transformation matrices to transform $\mathcal{B}_2$ to $\mathcal{R}$. Thus, these steps satisfy a strong backward error analysis in the sense of Bunch [6], i.e., there exists $\mathcal{E}_2 \in \mathbf{H}_{4n}$, such that

$$\tilde{\mathcal{U}}^T\mathcal{B}_2\tilde{\mathcal{U}} = \mathcal{R} + \mathcal{E}_2, \qquad \|\mathcal{E}_2\| \leq c_2\epsilon\,\|\mathcal{B}_2\| \leq c_2(1+c_1\epsilon)\epsilon\,\|\mathcal{H}\|\,.$$

Hence $\mathcal{U}^T\mathcal{B}\mathcal{U} = \mathcal{R} + \mathcal{E}$ with $\mathcal{E} = \mathcal{E}_2 + \tilde{\mathcal{U}}^T\mathcal{E}_1\tilde{\mathcal{U}} \in \mathbf{H}_{4n}$ and

$$\|\mathcal{E}\| \leq \|\mathcal{E}_2\| + \|\mathcal{E}_1\| \leq c\epsilon\,\|\mathcal{H}\|\,,$$

where $c = c_2(1+c_1\epsilon) + c_1$. $\square$

Lemma 4.4 *Consider the matrix $\mathcal{R} + \mathcal{E} \in \mathbf{H_{4n}}$ as in (40), (41), and let $\mathcal{Q}$ be as in (37). Then there exists $\mathcal{G} \in \mathbf{US}_{4n}$, and $Z_1, Z_2 \in \mathbf{U}_{2n}$ such that*

$$\mathcal{U} = \mathcal{Q}\,\mathrm{diag}(Z_1, Z_2)\mathcal{G}, \tag{42}$$

where $\mathcal{G}$ is such that

$$\mathcal{G}(\mathcal{R}+\mathcal{E})\mathcal{G}^T = \begin{bmatrix} \hat{R} & \hat{D} \\ 0 & -\hat{R}^T \end{bmatrix} =: \hat{\mathcal{R}}, \qquad \lambda(\hat{R}) = \lambda_+(\mathcal{B}), \tag{43}$$

and Z_1, Z_2 satisfy

$$\begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix} \hat{\mathcal{R}} \begin{bmatrix} Z_1 & 0 \\ 0 & Z_2 \end{bmatrix}^T = \begin{bmatrix} M & S \\ 0 & -M^T \end{bmatrix} := \mathcal{M} \tag{44}$$

with M, S defined by (38).

Proof. Since $\mathcal{H} \in \mathbf{H}^*_{2n}$ we have $\mathcal{B} \in \mathbf{H}^*_{4n}$. By (40) we have $\mathcal{R} + \mathcal{E} \in \mathbf{H}^*_{4n}$, so the Hamiltonian Schur form in (43) and hence the transformation matrix $\mathcal{G}$ exist.

Let $\mathcal{Z} = \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix} := \mathcal{Q}^T\mathcal{U}\mathcal{G}^T$, then (38), (40), and (43) imply that $\mathcal{Z}\hat{\mathcal{R}} = \mathcal{M}\mathcal{Z}$ with $\mathcal{M}$ as in (44). By comparing the $(2,1)$ blocks on both sides and recognizing that $\lambda(\hat{R}) = \lambda(M) = \lambda_+(\mathcal{B})$, it follows that $Z_{21} = 0$ and hence the orthogonality implies that $\mathcal{Z} = \mathrm{diag}(Z_1, Z_2)$ and thus the result follows. $\square$

Now we have prepared the ground for analysing the errors in the matrix Y computed by Algorithm 1. In order to simplify the presentation, in the following we do omit the analysis for Step 4 of Algorithm 1, since this analysis is well-known [12] and we assume that the columns of Y form an orthogonal basis of the left singular vector subspace of $\hat{Y}$, associated with the n largest singular values.

Theorem 4.5 *Let $\mathcal{M} = \mathcal{Q}^T\mathcal{B}\mathcal{Q} = \begin{bmatrix} M & S \\ 0 & -M^T \end{bmatrix} \in \mathbf{H}^*_{4n}$ be the Hamiltonian Schur form of $\mathcal{B}$ as in (38), let $\delta = \mathrm{Sep}(M^T, -M)$ be as in (39), and let $\mathcal{E}$ be the forward error matrix as in (40), (41). Furthermore, let Y be the exact output of Algorithm 1 and Y_ϵ the computed output* *in finite arithmetic. Denote by* $\Theta \in \mathbf{R}^{n\times n}$ *the diagonal matrix of canonical angles between* range$\{Y\}$ *and* range$\{Y_\epsilon\}$*. If*

$$8\,\|\mathcal{E}\|\,(\delta + \|S\|) < \delta^2, \tag{45}$$

then

$$\|\sin\Theta\| < c_s\frac{\|\mathcal{E}\|}{\delta} < c_s c\epsilon\frac{\|\mathcal{H}\|}{\delta}, \tag{46}$$

with $c_s = 8\,\dfrac{\sqrt{10}+4}{\sqrt{10}+2} \approx 11.1$.

Proof. Recognizing the block structures of $\hat{\mathcal{R}}$ and $\mathcal{M}$, (44) implies

$$Z_1\hat{R}Z_1^T = M, \qquad Z_2\hat{R}Z_2^T = M, \qquad Z_1\hat{D}Z_2^T = S.$$

Since Z_1, Z_2 are orthogonal, it follows that

$$\mathrm{Sep}(\hat{R}^T, -\hat{R}) = \delta, \qquad \|\hat{D}\| = \|S\|\,. \tag{47}$$

If we rewrite (43) as $\mathcal{G}^T(\hat{\mathcal{R}} + \hat{\mathcal{E}})\mathcal{G} = \mathcal{R}$, where $\hat{\mathcal{E}} = -\mathcal{G}\mathcal{E}\mathcal{G}^T$, then $\|\hat{\mathcal{E}}\| = \|\mathcal{E}\|$. Partition $\hat{\mathcal{E}} := \begin{bmatrix} \hat{E}_1 & \hat{E}_2 \\ \hat{E}_3 & -\hat{E}_1^T \end{bmatrix} \in \mathbf{H_{4n}}$ comformally to $\hat{\mathcal{R}}$. Then applying [27, Theorem V.2.5] it follows from (45) that

$$\mathrm{Sep}((\hat{R}+\hat{E}_1)^T, -(\hat{R}+\hat{E}_1)) \geq \mathrm{Sep}(\hat{R}^T, -\hat{R}) - 2\left\|\hat{E}_1\right\| \geq \delta - 2\,\|\mathcal{E}\| \geq 3\delta/4.$$

Inequality (45) implies that $\|\mathcal{E}\|\,\|S\| < \frac{\delta^2}{4} - \delta\,\|\mathcal{E}\|$. Adding $\|\mathcal{E}\|^2$ on both sides we obtain

$$\|\mathcal{E}\|\,(\|S\| + \|\mathcal{E}\|) < \frac{(\delta - 2\,\|\mathcal{E}\|)^2}{4},$$

which implies that

$$\|\hat{E}_3\|(\|\hat{D}\| + \|\hat{E}_2\|) < \frac{(\mathrm{Sep}(\hat{R}^T, -\hat{R}) - 2\|\hat{E}_1\|)^2}{4}. \tag{48}$$

Applying [27, Theorem V.2.7], there exists a symmetric matrix $W \in \mathbf{R}^{2n\times 2n}$ satisfying the algebraic Riccati equation

$$(\hat{R}+\hat{E}_1)^T W + W(\hat{R}+\hat{E}_1) + W(\hat{D}+\hat{E}_2)W - \hat{E}_3 = 0, \tag{49}$$

and

$$\|W\| \leq 2\|\hat{E}_3\|/(\delta - 2\|\hat{E}_1\|) < \frac{8}{3}\frac{\|\hat{E}_3\|}{\delta} < \frac{1}{3}, \tag{50}$$

where the last inequality follows from (45). (Note that in [27], Sep is defined using the Frobenius norm, the proof there is identical in spectral norm.) If we form

$$\hat{\mathcal{G}} := \begin{bmatrix} I_{2n} & -W \\ W & I_{2n} \end{bmatrix} \begin{bmatrix} (I_{2n}+W^2)^{-\frac{1}{2}} & 0 \\ 0 & (I_{2n}+W^2)^{-\frac{1}{2}} \end{bmatrix},$$

then $\hat{\mathcal{G}} \in \mathbf{US}_{4n}$, and

$$\tilde{\mathcal{R}} = \hat{\mathcal{G}}^T(\mathcal{R} + \hat{\mathcal{E}})\hat{\mathcal{G}} := \begin{bmatrix} \tilde{R} & \tilde{D} \\ 0 & -\tilde{R}^T \end{bmatrix}$$

with

$$\tilde{R} = (I + W^2)^{\frac{1}{2}}[\hat{R} + \hat{E}_1 + (\hat{D} + \hat{E}_2)W](I + W^2)^{-\frac{1}{2}}. \qquad (51)$$

We will prove that $\hat{\mathcal{G}}$ and $\mathcal{G}$ are essentially equal (up to a block orthogonal matrix which can be incorporated into $\mathrm{diag}(Z_1, Z_2)$ and will not affect the results). Since $\tilde{\mathcal{R}}$ is similar to $\mathcal{R}$ and $\lambda_-(R) = \emptyset$ (R is the upper left block of $\mathcal{R}$), it suffices to prove that $\lambda(\tilde{R}) = \lambda_+(\tilde{R})$, i.e., the spectrum of $\tilde{R}$ remains in the right half complex plane.

Let $t \in [0, 1]$ and $\mathcal{E}(t) = t\hat{\mathcal{E}}$, then clearly $\mathcal{E}(t)$ satifies (45). So from [27, Theorem V.2.11] for every matrix $\hat{\mathcal{R}} + \mathcal{E}(t)$, there exist a $W(t)$, the unique minimal norm solution of the Riccati equation analogous to (49), satisfying

$$\|W(t)\| < 2t\,\|\mathcal{E}\|/(\delta - 2t\,\|\mathcal{E}\|) < 1/3.$$

Hence, constructing $\hat{\mathcal{G}}(t)$ analogously it follows that $\hat{\mathcal{R}} + \mathcal{E}(t)$ is similar to a block upper triangular Hamiltonian matrix $\tilde{\mathcal{R}}(t) = \begin{bmatrix} \tilde{R}(t) & \tilde{D}(t) \\ 0 & -\tilde{R}(t)^T \end{bmatrix}$, with $\tilde{R}(t) = (I+W(t)^2)^{\frac{1}{2}} R_s(t)(I+W(t)^2)^{-\frac{1}{2}}$, and $R_s(t) := \hat{R} + t\hat{E}_1 + (\hat{D} + t\hat{E}_2)W(t)$. Condition (45) implies the bound (50) for $\|W(t)\|$ and then by elementary calculations it follows that for all $t \in [0, 1]$,

$$\mathrm{Sep}(R_s(t)^T, -R_s(t)) \geq \delta - 2\frac{\|\mathcal{E}\|\,(\delta + 2\,\|S\|)}{\delta - 2\,\|\mathcal{E}\|} > \frac{\delta}{2} > 0. \qquad (52)$$

The solutions $W(t)$ of the algebraic Riccati equation analogous to (49) with parameters depending on t is continuous in the coefficents, e.g., [18, Theorem 11.2.1] and also the eigenvalues of $R_s(t)$ and $\tilde{R}(t)$ are continuous in t.

Now suppose that some eigenvalues of $\tilde{R} = \tilde{R}(1)$ are in the closed left half complex plane. Then, by continuity, there must exist $t_0 \in [0, 1]$ such that $\lambda_0(\tilde{R}(t_0)) \neq \emptyset$. But this implies $\mathrm{Sep}(R_s(t_0)^T, -R_s(t_0)) = 0$, which contradicts (52).

Thus it follows that $\hat{\mathcal{G}} = \mathrm{diag}(V, V)\mathcal{G}$ for some $V \in \mathbf{U_{2n}}$ and by incorporating this block diagonal matrix into $\mathrm{diag}(Z_1, Z_2)$, we may assume that $\mathcal{G} = \hat{\mathcal{G}}$.

Recall the block forms of $\mathcal{Q}$, Q, $\mathcal{U}$ and the relations (37), (42). If we partition $Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix}$ with $Q_1, Q_2 \in \mathbf{R}^{2n \times n}$, then it follows that

$$\begin{aligned} \hat{Y} &:= \mathcal{U}_{21} - \mathcal{U}_{11} = Q(\begin{bmatrix} I_n & 0 \\ 0 & 0 \end{bmatrix} Z_1 - \begin{bmatrix} 0 & 0 \\ I_n & 0 \end{bmatrix} Z_2 W)(I_{2n} + W^2)^{-\frac{1}{2}} \\ &= (\begin{bmatrix} Q_1 & 0 \end{bmatrix} Z_1 - \begin{bmatrix} Q_2 & 0 \end{bmatrix} Z_2 W)(I_{2n} + W^2)^{-\frac{1}{2}}. \\ &= \begin{bmatrix} Q_1 & 0 \end{bmatrix} Z_1 + \begin{bmatrix} Q_1 & 0 \end{bmatrix} (Z_1(I_{2n} + W^2)^{-\frac{1}{2}} - I_{2n}) \\ &\quad - \begin{bmatrix} Q_2 & 0 \end{bmatrix} Z_2 W(I_{2n} + W^2)^{-\frac{1}{2}} \\ &=: \begin{bmatrix} Q_1 & 0 \end{bmatrix} Z_1 + E_Y. \end{aligned}$$

Performing some elementary calculations and using (50) we obtain

$$\begin{aligned} \|E_Y\| &\leq 1 - \frac{1}{\sqrt{1 + \|W\|^2}} + \frac{\|W\|}{\sqrt{1 + \|W\|^2}} \\ &< \frac{3\sqrt{10} + 12}{3\sqrt{10} + 10}\,\|W\| =: \rho\,\|W\| < \frac{\sqrt{10} + 4}{3\sqrt{10} + 10}. \end{aligned}$$

This means that $\hat{Y}$ can be considered as $\begin{bmatrix} Q_1 & 0 \end{bmatrix} Z_1$ perturbed by E_Y. Let the singular values of $\hat{Y}$ be given by $\sigma_1 \geq \cdots \geq \sigma_{2n} \geq 0$. Since the singular values of $\begin{bmatrix} Q_1 & 0 \end{bmatrix} Z_1$ are 1 and 0 both with multiplicity n, we have

$$\min_{1\leq k\leq n} \sigma_k \geq 1 - \|E_Y\|, \qquad \max_{n+1\leq k\leq 2n} \sigma_k \leq \|E_Y\|.$$

So

$$\eta := \min_{1\leq k\leq n} \sigma_k - \max_{n+1\leq k\leq 2n} \sigma_k \geq 1 - 2\|E_Y\| > \frac{\sqrt{10}+2}{3\sqrt{10}+10}.$$

Using the assumptions on Y and inequality (50), it follows by a result of Wedin (e.g., [27, Theorem V.4.4]) that

$$\|\sin\Theta\| \leq \frac{\|E_Y\|}{\eta} < \frac{\rho}{\eta}\|W\| < c_s\frac{\|\mathcal{E}\|}{\delta}$$

which is the first inequality of (46). The second inequality follows then from (41). $\square$

Remark 4.6 Assumption (45) usually is needed with a factor 4 instead of 8 in the literature. The factor 8 here is artificial, any other factor ≥ 4 that guarantees that $\eta > 0$ in the proof of Theorem 4.5 is sufficient.

Remark 4.7 $\mathrm{Sep}(T^T, -T)$ can be considered as a condition number for $\mathrm{Inv}_-(\mathcal{H})$. It is not difficult to see that $\mathrm{Sep}(\hat{T}, -\hat{T}^T)$ can be viewed as a condition number for $\mathrm{Inv}_+(\mathcal{H})$.

If $\mathrm{Sep}_2(T^T, -T) \approx \mathrm{Sep}_2(\hat{T}, -\hat{T}^T)$, then the bound (46) is similar to the bound obtained when the ideal strongly backwards stable algorithm would be used to compute the Hamiltonian Schur form. However, in general these two separations may be quite different. Consider the following example. Let

$$T = \begin{bmatrix} -\alpha & 1 \\ 0 & -\alpha \end{bmatrix}, \; R = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}, \; H = \begin{bmatrix} T & R \\ O & -T^T \end{bmatrix}.$$

Then

$$\hat{T} = \begin{bmatrix} -\alpha & \frac{-2\alpha}{\sqrt{1+4\alpha^2}} \\ 0 & -\alpha \end{bmatrix}.$$

If α is sufficiently small then $\mathrm{Sep}(T^T, -T) \approx 4\alpha^3$, while $\mathrm{Sep}(\hat{T}, -\hat{T}^T) \approx 2\alpha$. On the other hand, our algorithm computes both, $\mathrm{Inv}_-(\mathcal{H})$ and $\mathrm{Inv}_+(\mathcal{H})$, simultaneously. In this sense we conclude that our bound is essentially optimal, since both bounds are available.

5 Numerical Examples

In this section we present the numerical results obtained by applying Algorithm 1 to the problems of the benchmark collection for continuous-time algebraic Riccati equations [4] using the default parameters given there. The solutions of the algebraic Riccati equations are computed by solving the linear system $XU_{11} = -U_{21}$, where U_{11}, U_{21} are the $(1,1)$, $(2,1)$ blocks of $\mathcal{U}$ as returned from our new algorithm.

All examples were computed using MATLAB version 4.2c on a PC Pentium-s with IEEE standard double precision arithmetic and machine precision $\epsilon \approx 2.22 \times 10^{-16}$. (Note that

	E_X^1	E_X^2	R^1	R^2	E_λ^1	E_λ^2
1	0	2.1×10^{-16}	0	2.3×10^{-15}	2.2×10^{-16}	7.1×10^{-9}
2	4.7×10^{-15}	1.6×10^{-15}	3.9×10^{-13}	1.9×10^{-13}	8.9×10^{-16}	2.4×10^{-15}
3			1.4×10^{-14}	8.5×10^{-14}	2.9×10^{-15}	9.5×10^{-15}
4			9.0×10^{-15}	2.6×10^{-14}	3.6×10^{-15}	4.4×10^{-15}
5			7.3×10^{-14}	7.1×10^{-14}	3.7×10^{-13}	6.4×10^{-14}
6			1.3×10^{-4}	9.1×10^{-7}	1.6×10^{-8}	5.2×10^{-10}
7	8.3×10^{-5}	5.3×10^{-4}	3.3×10^{8}	2.1×10^{9}	6.7×10^{-16}	1.0×10^{0}
8			1.5×10^{-4}	4.1×10^{-3}	6.1×10^{-12}	9.7×10^{-9}
9	4.1×10^{-14}	4.1×10^{-14}	8.2×10^{-8}	8.2×10^{-8}	1.4×10^{-11}	1.4×10^{-11}
10	1.6×10^{-16}	7.2×10^{-2}	1.8×10^{-15}	1.0×10^{0}	2.7×10^{-17}	1.5×10^{-2}
11	2.1×10^{-8}	2.1×10^{-8}	2.5×10^{-9}	6.0×10^{-15}	4.0×10^{-10}	4.9×10^{-16}
12	5.7×10^{-4}	1.2×10^{0}	2.0×10^{16}	5.9×10^{18}	7.0×10^{-10}	6.1×10^{-2}
13			2.9×10^{-4}	2.4×10^{-4}	1.7×10^{-5}	1.2×10^{-5}
14			3.8×10^{-15}	1.7×10^{-15}	4.5×10^{-16}	4.5×10^{-16}
15			9.7×10^{-14}	1.1×10^{-13}	4.7×10^{-15}	4.7×10^{-15}
16			7.3×10^{-15}	2.8×10^{-13}	1.3×10^{-14}	1.3×10^{-14}
17	8.3×10^{-7}	6.6×10^{-7}	2.1×10^{3}	1.8×10^{3}	1.6×10^{-15}	1.6×10^{-15}
18			7.1×10^{-16}	7.1×10^{-16}	4.9×10^{-12}	4.9×10^{-12}
19			8.8×10^{-13}	1.1×10^{-12}	3.0×10^{-15}	3.0×10^{-15}

Table 2: Errors and Residuals of the Benchmark Examples

Example 20 from the benchmark collection is missing, since it requires more memory than available in the used computing environment.)

The results are shown in Table 2. There, X denotes the exact solution (if known) and $\hat{X}$ the solution computed with our new method. Furthermore, $E_X := \frac{\|\hat{X}-X\|_2}{\|X\|_2}$, provided X is known; in Example 17, we use $E_X = |\hat{x}_{n,1} - x_{n,1}|/|x_{n,1}|$ as it is the only available information about the exact solution. The 2-norm of the residual of the continuous-time algbraic Riccati equation (1) is denoted by R. Let $\mathcal{Y}$ be an orthogonal basis for Y computed by Algorithm 1 (determined via a rank revealing QR decomposition of $\hat{Y}$). If E_λ is the maximum eigenvalue error in $\mathcal{Y}^T\mathcal{H}\mathcal{Y}$, compared to $\lambda_-(\mathcal{H})$ computed by the symplectic URV method of [5], then E_λ can be viewed as a measure of the accuracy of the computed invariant subspace.

For each of the benchmark examples we ran the method twice, once the whole Algorithm 1 (superscript '1') and in the other case we stopped the algorithm after Step 2 (superscript '2') as discussed in Remark 3.5.

We compared the results with the result obtained using the Schur vector method as proposed in [19] and implemented in the MATLAB function `are` [22] and the multishift method as described in [2]. We refrain from reproducing all the data here. In general, Algorithm 1 produces errors of the same order as the other two methods. For the problems of larger dimension (Examples 15, 16, 18, 19), the new method produced the best results while the multishift method suffers from convergence problems and looses 1 to 3 orders of magnitude compared to Algorithm 1. Note that in Examples 6 and 11, the residual increases if the new method is not stopped after Step 2 while the residual after Step 2 is again of the same order as for the other two methods.

The large residuals in Examples 7, 12 and 17 are due to badly scaled algebraic Riccati equations. The relative errors obtained in these examples are in accordance with the condition of the matrix U_{11} which has to be factored in order to solve for X.

In Example 14, the solutions computed by Algorithm 1 and the Schur vector method are both nonsymmetric and the eigenvalues of $\hat{X}$ appear in complex conjugate pairs, while the multishift method yields the required symmetric solution. However, the symmetric parts $(\hat{X}^T + \hat{X})/2$ of the approximate solutions are also good approximations to X in this example, in the sense that the residuals are still of the same order.

Also note that in Example 11 the Hamiltonian matrix has eigenvalues on the imaginary axis causing the new method and the Schur vector method to loose half the number of significant digits while the multishift method computes the solution to full accuracy. From the other examples with eigenvalues close to the imaginary axis it seems that the multishift algorithm can handle this problem a little better (which can be explained by the fact that it is not affected by the conditioning of $Inv_+(\mathcal{H})$, i.e., $\mathrm{Sep}(\hat{T}, -\hat{T}^T)$). On the other hand, the new method overcomes the problems of the multishift method for growing dimensions while still being substantially faster than the Schur vector method.

The method to stop after Step 2 of Algorithm 1 breaks down in Example 10. In this case, one computes a basis of an invariant subspace of dimension one (while the desired subspace has dimension two).

6 Conclusion

We have presented a new method for the computation of Lagrangian invariant subspaces of real Hamiltonian matrices. By embedding the matrix into a specially structured Hamiltonian matrix of double size, we can compute the desired subspace via a method that is not only backward stable, but has a forward error of Hamiltonian structure and thus reflects the structure of the problem in a sufficient way.

The complexity of the method is less than that of the standard QR-algorithm with eigenvalue reordering. It works very well for problems in $\mathbf{H}_{\mathbf{2n}}^{*}$ and it can in principle also be applied to problems with eigenvalues on the imaginary axis, but currently it is not clear which subspace one should compute then.

Appendix

In this Appendix we give an alternative method for the computation of U_3 in Step 2 of Algorithm 1. This method makes use of the special structure of H_b and H_t. The symplectic URV decomposition yields block-matrices $H_t = [H^t_{ij}]_{s\times s}, H_b = [H^b_{ij}]_{s\times s} \in \mathbf{R}^{n\times n}$ partitioned analogously, where H^t_{ii}, H^b_{ii} are $n_i \times n_i$, $i = 1, 2, \ldots, s$. We want to transform $\begin{bmatrix} 0 & H_b \\ H_t & 0 \end{bmatrix}$ to quasi upper triangular form using a finite sequence of orthogonal tranformations. As in the common reordering of the real Schur form using the Bartels-Stewart algorithm, e.g., [12], we need to distinguish different cases depending on the size (1×1 or 2×2) of the blocks we treat. We have to solve the following elementary problems:

1. For nonnegative scalars K, L or 2×2 matrices K, L such that KL has a pair of complex conjugate eigenvalues find an orthogonal matrix Z such that

$$Z^T \begin{bmatrix} 0 & L \\ K & 0 \end{bmatrix} Z =: \begin{bmatrix} T_1 & T_3 \\ 0 & -T_2 \end{bmatrix}, \tag{53}$$

with $\lambda(T_1) = \lambda(T_2)$ and $\lambda_-(T_1) = \emptyset$.
In the 1×1 case let

$$Z = \begin{bmatrix} c & s \\ -s & c \end{bmatrix},$$

with

$$c := \sqrt{\frac{L}{L+K}}, s := -\sqrt{\frac{K}{L+K}},$$

then

$$Z^T \begin{bmatrix} 0 & L \\ K & 0 \end{bmatrix} Z = \begin{bmatrix} \sqrt{KL} & L-K \\ 0 & -\sqrt{KL} \end{bmatrix} =: \begin{bmatrix} T_1 & T_3 \\ 0 & -T_2 \end{bmatrix}.$$

For the 2×2 case we first determine the eigenvalues with positive real parts of the matrix $\begin{bmatrix} 0 & L \\ K & 0 \end{bmatrix}$. They are $a \pm ib$, $a > 0$, with

$$\begin{aligned} a &= \tfrac{1}{2}\sqrt{2\sqrt{\det(KL)} + \operatorname{trace}(KL)}, \\ b &= \tfrac{1}{2}\sqrt{2\sqrt{\det(KL)} - \operatorname{trace}(KL)}. \end{aligned}$$

We then apply the QR algorithm with double shifts $a \pm ib$ (e.g. [12]) to $\begin{bmatrix} 0 & L \\ K & 0 \end{bmatrix}$. Since the matrix size is 4×4 and since the shifts are very close to the accurate ones, usually one or two iterations are sufficient to get (53).

2. For a given matrix $\begin{bmatrix} T_1 & 0 \\ T_3 & -T_2 \end{bmatrix}$, where T_1 and T_2 are either 1×1 or 2×2, determine an orthogonal matrix Z such that

$$Z^T \begin{bmatrix} T_1 & 0 \\ T_3 & -T_2 \end{bmatrix} Z =: \begin{bmatrix} \tilde{T}_1 & \tilde{T}_3 \\ 0 & -\tilde{T}_2 \end{bmatrix}, \tag{54}$$

where $\lambda(T_1) = \lambda(\tilde{T}_1)$ and $\lambda(T_2) = \lambda(\tilde{T}_2)$. If both T_1, T_2 are 1×1, then we form

$$Z = \begin{bmatrix} c & s \\ -s & c \end{bmatrix},$$

with

$$c := \frac{T_1 + T_2}{\sqrt{T_3^2 + (T_1 + T_2)^2}}, \quad s := -\frac{T_3}{\sqrt{T_3^2 + (T_1 + T_2)^2}}.$$

Then

$$Z^T \begin{bmatrix} T_1 & 0 \\ T_3 & -T_2 \end{bmatrix} Z = \begin{bmatrix} T_1 & -T_3 \\ 0 & -T_2 \end{bmatrix}.$$

If at least one of T_1 or T_2 is 2×2, then we obtain (54) by applying the QR algorithm with the eigenvalue(s) of $-T_2$ as the shift(s). Again one or two iterations are usually sufficient.

Algorithm 2

Input: *Real $n \times n$ matrices H_t, H_b with H_t upper triangular and H_b quasi upper triangular.*

Output: $U_3 \in \mathbf{U}_{2n}$, *Δ as in (31) and Π_3 as in (33).*

% Initialize U_3.

Set $U = I_{2n} := \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}$.

FOR $i = 1, \ldots, s$

Set $C(i:s) = 0$, $D(i:s) = H_b(i, i:s)$, $H_b(i, i:s) = 0$.
% Store Δ in H_b.

FOR $j = i, i-1, \ldots, 1$
IF $j = i$ *THEN*
% Annihilate $H_t(j, j)$.
Take $H_t(j, j)$, $D(i)$ as K, L of (53). Determine the orthogonal matrix

$$Z := \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix},$$

such that

$$Z^T \begin{bmatrix} 0 & L \\ K & 0 \end{bmatrix} Z =: \begin{bmatrix} T_1 & T_3 \\ 0 & -T_2 \end{bmatrix},$$

ELSE
% Annihilate $H_t(j, i)$.
Take $H_t(j, i)$, $C(i)$, $H_b(j, j)$ as T_3, T_1, T_2 in (54). Determine the orthogonal matrix

$$Z := \begin{bmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{bmatrix}$$

such that

$$Z^T \begin{bmatrix} T_1 & 0 \\ T_3 & -T_2 \end{bmatrix} Z =: \begin{bmatrix} T_1 & T_3 \\ 0 & -T_2 \end{bmatrix}.$$

END IF

Set

$$\begin{aligned}
C(i) &:= T_1, \qquad D(j) := T_3, \\
H_t(j,i) &:= 0, \qquad H_b(j,j) := T_2, \\
C(i+1:s) &:= Z_{11}^T C(i+1:s) + Z_{21}^T H_t(j,i+1:s), \\
H_t(j,i+1:s) &:= Z_{12}^T C(i+1:s) + Z_{22}^T H_t(j,i+1:s), \\
D(j+1:s) &:= Z_{11}^T D(j+1:s) - Z_{21}^T H_b(j,j+1:s), \\
H_b(j,j+1:s) &:= -Z_{12}^T D(j+1:s) + Z_{22}^T H_b(j,j+1:s), \\
H_t(1:j-1,i) &:= H_t(1:j-1,i) Z_{11} - H_b(1:j-1,j) Z_{21}, \\
H_b(1:j-1,j) &:= -H_t(1:j-1,i) Z_{12} + H_b(1:j-1,j) Z_{22}; \\
U_{11}(j:i,i) &:= U_{11}(j:i,i) Z_{11} + U_{12}(j:i,j) Z_{21}, \\
U_{12}(j:i,j) &:= U_{11}(j:i,i) Z_{12} + U_{12}(j:i,j) Z_{22}, \\
U_{21}(j:i,i) &:= U_{21}(j:i,i) Z_{11} + U_{22}(j:i,j) Z_{21}, \\
U_{22}(j:i,j) &:= U_{21}(j:i,i) Z_{12} + U_{22}(j:i,j) Z_{22}.
\end{aligned}$$

END FOR j

END FOR i

% Form Π_3 *as in (33) and store it in* H_r.

$H_r := U_{22}^T H_r U_{12}$, $H_r := H_r + H_r^T$.

END

References

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

[2] 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.

[3] G.S. Ammar, W. B. Gragg, and L. Reichel. On the eigenproblem for orthogonal. In *Proc. 25th IEEE Conference on Decision and Control*, pages 1963–1966, 1986.

[4] 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. Available as `SPC95_22.ps` via anonymous ftp from `ftp.tu-chemnitz.de`, directory `/pub/Local/mathematik/Benner`.

[5] P. Benner, V. Mehrmann, and H. Xu. A numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian or symplectic pencils. Technical Report SFB393/96-06, Fak. f. Mathematik, TU Chemnitz–Zwickau, 09107 Chemnitz, FRG,

1996. Available as SFB393_96-05.ps via anonymous ftp from ftp.tu-chemnitz.de, directory /pub/Local/mathematik/Benner. Submitted for publication.

[6] J.R. Bunch. The weak and strong stability of algorithms in numerical algebra. *Linear Algebra Appl.*, 88:49–66, 1987.

[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] R. Byers. *Hamiltonian and Symplectic Algorithms for the Algebraic Riccati Equation.* PhD thesis, Cornell University, Dept. Comp. Sci., Ithaca, NY, 1983.

[10] R. Byers. A Hamiltonian QR-algorithm. *SIAM J. Sci. Statist. Comput.*, 7:212–229, 1986.

[11] T. Chan. Rank revealing QR factorizations. *Linear Algebra Appl.*, 88/89:67–82, 1987.

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

[13] W. B. Gragg. The QR algorithm for unitary hessenberg matrices. *J. Comp. Appl. Math.*, 16:1–8, 1968.

[14] W. B. Gragg and L. Reichel. A divide and conquer algorithm for the unitary and orthogonal eigenproblem. *Numer. Math*, 57:695–718, 1990.

[15] G.A. Hewer and C. Kenney. The sensitivity of the stable Lyapunov equation. *SIAM J. Cont. Optim.*, 26:321–344, 1988.

[16] N. J. Higham. The matrix sign decomposition and its relation to the polar decomposition. *Linear Algebra Appl.*, 212/213:3–20, 1994.

[17] R.A. Horn and C.R. Johnson. *Matrix Analysis.* Cambridge University Press, Cambridge, 1985.

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

[19] 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).

[20] 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.

[21] W.-W. Lin and T.-C. Ho. On Schur type decompositions for Hamiltonian and symplectic pencils. Technical report, Institute of Applied Mathematics, National Tsing Hua University, Taiwan, 1990.

[22] The MATLAB Control Toolbox. The MathWorks, Inc., Cochituate Place, 24 Prime Park Way, Natick, Mass, 01760, 1990.

[23] 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.

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

[25] B.N. Parlett. *The Symmetric Eigenvalue Problem.* Prentice-Hall, Englewood Cliffs, NJ, 1980.

[26] J.D. Roberts. Linear model reduction and solution of the algebraic Riccati equation by use of the sign function. *Internat. J. Control*, 32:677–687, 1980. (Reprint of Technical Report No. TR-13, CUED/B-Control, Cambridge University, Engineering Department, 1971).

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

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

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

[30] H. Xu. *Solving Algebraic Riccati Equations via Skew-Hamiltonian Matrices.* PhD thesis, Inst. of Math., Fudan University, Shanghai, P.R. China, April 1993.

[31] H. Xu and L. Lu. Properties of a quadratic matrix equation and the solution of the continuous-time algebraic Riccati equation. *Linear Algebra Appl.*, 222:127–146, 1995.