A NEW METHOD FOR THE HAMILTONIAN EIGENVALUE PROBLEM

Peter Benner, Volker Mehrmann, and Hongguo Xu

Fakultät für Mathematik
TU Chemnitz-Zwickau
D-09107 Chemnitz (FRG)
Fax.: +49 371 5312657 and e-mail: hxu@mathematik.tu-chemnitz.de

Abstract

A new method is presented for the numerical computation of the eigenvalues of real Hamiltonian matrices. The method is strongly backward stable, i.e., it is numerically backward stable and preserves the Hamiltonian structure. It 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 ε is the machine precision, the new method computes the eigenvalues to full possible accuracy.

Keywords: Numerical Methods, Linear Systems, Optimal Control

1 Introduction

A matrix $\mathcal{H} \in \mathbf{R}^{2n\times 2n}$ is called **Hamiltonian** iff $(\mathcal{H}J)^T = \mathcal{H}J$, where $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$. The Lie Algebra of Hamiltonian matrices in $\mathbf{R}^{2n\times 2n}$ is denoted by $\mathbf{H_{2n}}$. The problem of computing the eigenvalues of Hamiltonian matrices is very important in many applications in control theory and signal processing, see, e.g., [13, 11].

It is still an open problem to find a completely satisfactory method to compute the eigenvalues and the invariant subspace corresponding to the eigenvalues in the open left half plane. 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 structure. Many attempts have been made to tackle this problem, see [7, 12, 13] but 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, [1].

If only the eigenvalues are required (these are the closed loop eigenvalues), the situation is different. These can for example be obtained via the square-reduced method of Van Loan [14]. This method is 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 [14].

In this paper we will present a new method which does not suffer from this loss of accuracy. The method is structure preserving, backward stable, and needs $O(n^3)$ floating point operations. Its computational cost is significantly lower than the cost for computing the eigenvalues of a Hamiltonian matrix by the standard QR algorithm as given, e.g., in [8]. The main ingredients for the new method are a new matrix decomposition, which can be viewed as a symplectic URV decomposition, and a periodic Schur decomposition for the product of two matrices.

The method uses non-similarity transformations with orthogonal symplectic matrices. 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 $\mathbf{US_{2n}}$.

2 Theoretical Background

The basis for our new algorithm is a non-similarity transformation for the original Hamiltonian matrix, which leads to a similarity transformation for the skew-Hamiltonian matrix $\mathcal{H}^2$. From the eigenvalues of $\mathcal{H}^2$ we can then easily compute the eigenvalues of $\mathcal{H}$. If we would form $\mathcal{H}^2$ directly or indirectly as in the square reduced method [14], we would suffer from the same possible $\sqrt{\varepsilon}$ perturbation in the computed eigenvalues as in Van Loan's method. But in this situation we can apply a trick that is based on a non-similarity transformation.

Theorem 1 *Let $A \in \mathbf{R}^{2n\times 2n}$. Then there exist matrices $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that*

$$Q_1^T A Q_2 = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}, \tag{1}$$

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

Proof. See [5]. □

At first sight it is not clear how the above transformation can be used for eigenvalue computation, but when we apply the transformation to a Hamiltonian matrix we obtain the following corollary.

Corollary 2 *Let $\mathcal{H} \in \mathbf{H_{2n}}$. Then there exist $Q_1, Q_2 \in \mathbf{US_{2n}}$ such that*

$$
\begin{aligned}
Q_1^T \mathcal{H}^2 Q_1 &= \begin{bmatrix} -H_{11}H_{22}^T & H_{11}H_{12}^T - H_{12}H_{11}^T \\ 0 & -H_{22}H_{11}^T \end{bmatrix}, \\
Q_2^T \mathcal{H}^2 Q_2 &= \begin{bmatrix} -H_{22}^T H_{11} & H_{12}^T H_{22} - H_{22}^T H_{12} \\ 0 & -H_{11}^T H_{22} \end{bmatrix},
\end{aligned}
$$

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

From this result we see that in order to compute the eigenvalues of a Hamiltonian matrix it suffices to compute the eigenvalues of

$$-H_{11}H_{22}^T \quad \text{or} \quad -H_{22}^T H_{11}. \tag{2}$$

Now fortunately we can compute the eigenvalues of (2) without forming the products. To do this we can employ the periodic Schur decomposition for products of matrices [6, 9, 10] without forming the products. The periodic QR algorithm applied to the second product of (2) yields real orthogonal transformation matrices $U, V \in \mathbf{R}^{n\times n}$ such that

$$\hat{H} := -U^T H_{22}^T V V^T H_{11} U, \qquad \hat{H}_{22}^T := (V^T H_{22} U)^T \tag{3}$$

are quasi-upper triangular, while

$$\hat{H}_{11} := V^T H_{11} U \tag{4}$$

is upper triangular. After these forms have been computed, we can compute the eigenvalues of $\hat{H}$ by solving 1×1 or 2×2 eigenvalue problems.

Remark 1 Note that the described procedure cannot be applied to complex Hamiltonian matrices. 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 [14].

3 The Numerical Algorithm

We have already described the main features of the new algorithm in Section 2.

Algorithm 1 *A structure preserving method for the computation of the eigenvalues of a Hamiltonian matrix.*
Input: A Hamiltonian matrix $\mathcal{H} \in \mathbf{H_{2n}}$.
Output: The eigenvalues $\{\gamma_1, \ldots, \gamma_{2n}\}$ of $\mathcal{H}$.
Step 1: Determine $Q_1, Q_2 \in \mathbf{US_{2n}}$, such that

$$Q_1^T \mathcal{H} Q_2 = \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix}, \tag{5}$$

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 [9] to the product matrix

$$-H_{22}^T H_{11}, \tag{6}$$

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

$$V^T H_{11} U =: \hat{H}_{11}, \tag{7}$$

is upper triangular and

$$(V^T H_{22} U)^T =: \hat{H}_{22}^T \tag{8}$$

is quasi-upper triangular.
Step 3: Solve the 1×1 or 2×2 eigenvalue problems arising from explicitly multiplying out the diagonal blocks in (7), (8), i.e., determine eigenvalues λ_i, $i = 1, \ldots, n$, via the solution of the 1×1 or 2×2 eigenvalue problems arising in the block diagonal of the product $-\hat{H}_{11}\hat{H}_{22}^T$.
Step 4: Compute the eigenvalues of $\mathcal{H}$ by

$$\gamma_i = \sqrt{\lambda_i}, \quad \gamma_{n+i} = -\sqrt{\lambda_i}, \qquad i = 1, \ldots, n.$$

End

The reduction to the condensed form (5) is described in detail in [5]. The computational cost is comparable to reducing a $2n\times 2n$ real matrix to Hessenberg form by Householder reflections. The cost for computing the periodic Schur decomposition as proposed in [9] of the product of a Hessenberg matrix with an upper-triangular matrix is about three times the cost for applying the standard QR iteration (see, e.g., [8]) to the product. Altogether, Algorithm 1 requires about $48n^3$ flops[1] as opposed to $80n^3$ flops for the standard QR algorithm applied to $\mathcal{H}$. That is, the new method is significantly cheaper than the standard QR algorithm. On the other hand, the square-reduced method of Van Loan [14] as implemented in [3] requires about $29n^3$ flops which is less than two thirds of the computational cost for the new method. But the benefit of the increase in computational cost is the more favorable error analysis presented in the next section.

4 Error Analysis

In this section, we will derive the error analysis for Algorithm 1.

Since all transformations are performed with orthogonal and orthogonal symplectic matrices we can apply the standard backward error analysis of Wilkinson, e.g., [16, 8]. Using the usual arguments in the analysis of orthogonal transformations, e.g., [16, 8], we obtain that there exists a $2n\times 2n$ matrix E with $\|E\| \approx \varepsilon\,\|\mathcal{H}\|$, where ε denotes the

[1] Following [8], we define each floationg point arithmetic operation ('+', '−', '*', '/', '$\sqrt{\ }$') as a **flop**.

machine precision, such that the factorization computed by Algorithm 1 satisfies

$$\hat{\mathcal{H}} := \begin{bmatrix} H_{11} & H_{12} \\ 0 & H_{22} \end{bmatrix} = \hat{\mathcal{U}}_1^T(\mathcal{H} + E)\hat{\mathcal{U}}_2 \tag{9}$$

with H_{11} upper triangular and H_{22} quasi-lower triangular. Here, $\hat{\mathcal{U}}_1, \hat{\mathcal{U}}_2 \in \mathbf{US_{2n}}$ denote the accumulated orthogonal symplectic transformations performed by Algorithm 1 in finite-precision arithmetic.

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 (9), $\hat{\lambda}^2$ is also an eigenvalue of $(\mathcal{H}+JE^TJ)(\mathcal{H}+E)$.

The *condition* of a simple eigenvalue λ of a matrix $A \in \mathbf{R}^{n\times n}$ as defined in [16] is given by

$$\frac{1}{s(\lambda)} = \frac{1}{|y^H x|} \tag{10}$$

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

Theorem 3 *Let λ 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 (10). Let ε be the machine precision. If the matrix E in (9) satisfies $\|E\| < \varepsilon\|\mathcal{H}\|$, and*

$$\frac{2\|\mathcal{H}\|\varepsilon}{|\lambda|s(\lambda)} < 1,$$

then Algorithm 1 yields a computed eigenvalue $\hat{\lambda}$ such that

$$\begin{aligned} |\hat{\lambda} - \lambda| &\leq \frac{\|\mathcal{H}\|\varepsilon}{(1 - \frac{\|\mathcal{H}\|\varepsilon}{|\lambda|s(\lambda)})s(\lambda)} + O(\varepsilon^2) \\ &\leq \frac{2\|\mathcal{H}\|\varepsilon}{s(\lambda)} + O(\varepsilon^2). \end{aligned}$$

Proof. See [5]. □

As a consequence of Theorem 3 we have that Algorithm 1 is numerically backward stable.

Remark 2 From the error analysis in Theorem 3 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 3, the prize is an increase in computational cost.

5 Numerical Examples

Algorithm 1 was implemented in Fortran 77 and was tested for all examples given in the benchmark collections for continuous-time algebraic Riccati equations [4], the examples given in [14], and some randomly generated examples. Here, we present only the experiment for the worst case example of [14] and some timings.

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`.

We compared the following methods:

- **ALG 1**, the new method as given in Algorithm 1 using the periodic Schur decomposition [9] as implemented in [15],
- **SQRED**, Van Loan's square reduced method as implemented in [3],
- **LAPACK**, nonsymmetric eigenproblem solver DGEEVX from LAPACK [2].

All subroutines use the BLAS and LAPACK [2] as far as possible.

Example 1 [14, 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 three methods.

λ	ALG 1	SQRED	LAPACK
1	0	0	7.8×10^{-16}
10^{-2}	5.5×10^{-16}	5.5×10^{-16}	5.0×10^{-17}
10^{-4}	1.6×10^{-18}	1.6×10^{-14}	2.6×10^{-18}
10^{-6}	1.0×10^{-18}	1.5×10^{-11}	8.4×10^{-18}
10^{-8}	3.1×10^{-17}	2.2×10^{-9}	4.7×10^{-17}

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

From Table 1 the loss of accuracy of $\|H\|/|\lambda|$ for Van Loan's method is obvious. As to be expected, the same loss of accuracy can be observed if the reduction of Corollary 2 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 2 We tested the three 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 three 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 2 are the mean values of the CPU times measured on a HP Model 712/60 work station.

n	ALG 1	SQRED	LAPACK
25	0.095	0.062	0.146
50	0.57	0.34	0.77
75	1.77	1.04	2.41
100	4.25	2.58	5.76
125	8.03	5.01	11.25
150	13.18	8.37	19.22
175	20.49	13.05	29.57
200	30.07	19.33	45.15

Table 2: Example 2, CPU times

Table 2 shows that both Algorithm 1 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 to the fact that both methods are more complex as far as index handling, memory access, and subroutine calls are concerned. Besides, DGEEVX does not implement the standard QR algorithm as described in [8], but is modified in several aspects. Our new method and the square reduced method of Van Loan use the Hamiltonian structure and thus return the right pairing of eigenvalues. The QR algorithm treats a Hamiltonian matrix like an arbitrary nonsymmetric matrix. Therefore, small perturbations can cause computed eigenvalues with small imaginary part to cross the imaginary axis. For instance, for $n = 100$ DGEEVX returned between 95 and 103 eigenvalues with negative real part.

6 Conclusions

We have presented a new method for computing the eigenvalues of Hamiltonian matrices. The method is numerically strongly backward stable since it preserves the underlying Hamiltonian structure and uses only backward stable orthogonal transformations. The algorithm saves a significant amount of computational cost compared to the standard QR algorithm. On the other hand, the new method is more expensive in both computational cost and work space than Van Loan's method, but does not suffer from the possible $O(\sqrt{\varepsilon})$ loss of accuracy as this methods does.

Similar techniques can be used to compute the eigenvalues of Hamiltonian pencils and, employing Cayley transformations, also for symplectic matrices and pencils. The error analysis shows that the method is numerically strongly backward stable for all these problems.

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