ON THE IWASAWA DECOMPOSITION OF A SYMPLECTIC MATRIX

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Abstract. We consider the computation of the Iwasawa decomposition of a symplectic matrix via the QR factorization. The algorithms presented improve on the method recently decribed in [8].

Key words. Iwasawa decomposition, symplectic group, QR factorization

1. Introduction. A matrix $S \in \mathbb{R}^{2n\times 2n}$ is called *symplectic* if it satisfies $S^tJS = J$, where

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}.$$

In this note we are concerned primarily with the real case; the complex case can be treated along similar lines. Under matrix multiplication, the symplectic matrices form a (non-compact) Lie group denoted by $\mathcal{S} = Sp(n,\mathbb{R}) = \{S \in SL_{2n}(\mathbb{R}) : S^tJS = J\}$, where $SL_{2n}(\mathbb{R})$ denotes the group of $2n \times 2n$ matrices with unit determinant. The symplectic group is closed under transposition. Consider the following subgroups of $\mathcal{S}$:

$$\mathcal{K} = \left\{ K = \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix} : K_{11} + iK_{12} \in U(n) \right\} = O(2n) \cap Sp(n,\mathbb{R}),$$
$$\mathcal{A} = \left\{ \begin{pmatrix} A_{11} & 0 \\ 0 & A_{11}^{-1} \end{pmatrix} : A_{11} \text{ positive diagonal} \right\},$$
$$\mathcal{N} = \left\{ \begin{pmatrix} N_{11} & N_{12} \\ 0 & N_{11}^{-t} \end{pmatrix} : N_{11} \text{ unit upper triangular, } N_{11}N_{12}^t = N_{12}N_{11}^t \right\}.$$

The first of these three subgroups is compact, the second is abelian, and the third is nilpotent. The decomposition $\mathcal{S} = \mathcal{KAN}$ is called the *Iwasawa decomposition* of $\mathcal{S}$. Any $S \in Sp(n,\mathbb{R})$ can be written as $S = KAN$, where $K \in \mathcal{K}$, $A \in \mathcal{A}$, and $N \in \mathcal{N}$; moreover, this decomposition is unique. It is a special case of the general Iwasawa decomposition of a connected semisimple Lie group first given in [7]. For a more detailed discussion of the Iwasawa decomposition, see [9] or [5]. The importance of this decomposition is both theoretical and practical, in particular in the area of dynamical systems. Note that the factorization $S = KAN$ (more precisely, the factorization $S = KM$ with $M = AN$) differs from the QR factorization [10], since N is not upper triangular. (Note that the factors in the usual QR factorization of S are not symplectic, in general.) It is also not to be confused with the *SR factorization* (see, e.g., [3, p. 20]). The decomposition $S = KM$ with $M = AN$ is called a *unitary SR decomposition* in [2, pp. 68–69].

In the recent note [8], Tam presents an algorithm and MATLAB code for explicitly computing the Iwasawa decomposition $S = KAN$ of a symplectic matrix using the Cholesky factorization of S^tS. Unfortunately, this algorithm is problematic in many

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ways from a computational point of view, and furthermore the MATLAB code in [8] is incorrect. With the present note we intend to rectify these problems.

2. Computing the Iwasawa decomposition. The approach in [8] is based on the following result.

THEOREM 2.1. *Let* $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \in \mathcal{S}$ *and* $S^tS = \begin{pmatrix} A_1 & B_1 \\ B_1^t & D_1 \end{pmatrix}$ *(also in* $\mathcal{S}$*). Let* $A_1 = U^tHU$ *be the root-free Cholesky factorization of the symmetric positive definite matrix* A_1*, where* U *is unit upper triangular and* H *is positive diagonal. Then* $S = KAN$*, where*

$$A = \begin{pmatrix} H^{\frac{1}{2}} & 0 \\ 0 & H^{-\frac{1}{2}} \end{pmatrix}, \quad N = \begin{pmatrix} U & H^{-1}U^{-t}B_1 \\ 0 & U^{-t} \end{pmatrix}, \quad \text{and} \quad K = S(AN)^{-1},$$

is the Iwasawa decomposition of S*.*

Based on Theorem 2.1, the author of [8] proposes a Cholesky-based algorithm and a MATLAB implementation for explicitly determining the Iwasawa factors K, A, N of a given symplectic matrix. This approach suffers from several drawbacks. To begin with, the MATLAB code in [8] contains a mistake in the way the root-free Cholesky factor of A_1 is obtained from the standard Cholesky factorization; as a result, the computed factors K, A, N are very far from the actual Iwasawa factors. In particular, the computed K is not orthogonal, in general. Correcting the mistake results in a formally correct algorithm which, however, suffers from potential numerical instabilities. It is well known that forming the product S^tS explicitly may lead to significant loss of information in finite precision computations; see [6, p. 386]. If S is ill-conditioned (which can happen, since the group $\mathcal{S}$ is not compact), forming S^tS may even result in loss of positive definiteness, with the consequent breakdown of the Cholesky factorization. Although efficiency is not the primary concern of this note, it is also worth noting that forming the entire product S^tS when only the first n columns of it are needed is wasteful and can be easily avoided.

Another concern lies in the repeated usage of the function `inv` in the MATLAB code in [8]. These matrix inversions are another potential source of instability, are inefficient, and can be easily avoided. Finally, the implementation in [8] contains some redundancies (the same matrix products are performed repeatedly).

We can extract from [2, pp. 64–69] a method for computing the Iwasawa decomposition of a symplectic matrix, which proceeds as follows. Given a real symplectic matrix $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$, the following algorithm computes the factors K, A, N of the Iwasawa decomposition of S.

ALGORITHM 2.2.

1. *Compute the QR factorization of* $S_{11} + iS_{12}$*; denote by* U *the unitary factor of* $S_{11} + iS_{12}$*.*
2. *Compute the Iwasawa factors* K*,* A *and* N *of* S *as follows:*

$$\begin{aligned}
&K_{11} = \tfrac{1}{2}(U + \bar{U}), \quad K_{12} = \tfrac{i}{2}(\bar{U} - U),\\
&K \;\; = \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix},\\
&\hat{N} \;\; = K^tS\\
&A \;\; = \operatorname{diag}(\hat{n}_{11}, \ldots, \hat{n}_{2n,2n}), \text{ where } \hat{n}_{ii} \text{ are the diagonal entries of } \hat{N},\\
&N \;\; = A^{-1}\hat{N}.
\end{aligned}$$

Note that Algorithm 2.2 necessitates complex arithmetic even if the symplectic matrix S and its factors are real, an undesirable feature. Motivated by this, we examine here another algorithm for computing the Iwasawa decomposition of a symplectic matrix. This approach is based on the "thin" QR factorization [4, p. 230] and does not require complex arithmetic. Let S be partitioned into four blocks as in Theorem 2.1. The following algorithm computes the factors K, A, N in the Iwasawa decomposition of S.

Algorithm 2.3.

1. *Let* $S_1 = \begin{pmatrix} S_{11} \\ S_{21} \end{pmatrix}$.
2. *Compute the thin QR factorization of* S_1, *where* $Q = \begin{pmatrix} Q_{11} \\ Q_{21} \end{pmatrix}$ *and* $R = R_{11}$.
3. *Factor the upper triangular matrix* R_{11} *as* $R_{11} = HU$ *with* H *diagonal and* U *unit upper triangular. Then* $R_{11}^t R_{11} = U^t D U$, *where* $D = H^2$.
4. *Compute the Iwasawa factors* A, K *and* N *of* S *as follows:*

$$\begin{aligned} A &= \begin{pmatrix} D^{\frac{1}{2}} & 0 \\ 0 & D^{-\frac{1}{2}} \end{pmatrix} \in \mathcal{A}, \\ K_{11} &= Q_{11} H D^{-\frac{1}{2}}\ , \quad K_{12} = -Q_{21} H D^{-\frac{1}{2}}, \\ K &= \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix} \in \mathcal{K}, \\ N &= \begin{pmatrix} U & N_{12} \\ 0 & N_{22} \end{pmatrix} \in \mathcal{N}\ , \ \textit{where} \begin{pmatrix} N_{12} \\ N_{22} \end{pmatrix} = A^{-1} K^t \begin{pmatrix} S_{12} \\ S_{22} \end{pmatrix}. \end{aligned}$$

A few remarks are in order. Since $D = H^2$, the matrix $HD^{-\frac{1}{2}}$ appearing in step 4 is just a signature matrix, i.e., a diagonal matrix with entries equal to ± 1. The above algorithm requires no explicit matrix inverses except for that of a diagonal matrix. The cost of the algorithm is dominated by the computation of the QR factorization of S_1 and by the matrix products in the computation of N_{12} and N_{22}. We point out that the overall cost of Algorithm 2.3 is $\frac{40}{3}n^3 + O(n^2)$ floating point operations, which is less than the explicit computation of $S^t S$ (the cost of which is $16n^3$ floating point operations). Therefore, the cost of Algorithm 2.3 is significantly less than the cost of the algorithm in [8]. We also note that the use of complex arithmetic in Algorithm 2.2 makes this approach significantly more expensive than Algorithm 2.3 in the real case. It is quite possible that even more efficient algorithms could be developed, for instance making use of the symplectic QR decomposition described in [1]. Here we restrict ourselves to algorithms that can be easily implemented in Matlab using only built-in functions.

3. Numerical experiments. We constructed a number of symplectic matrices of different dimensions by first constructing the symplectic Iwasawa factors K, A and N and then forming the product $S = KAN$. Specifically, we constructed the blocks for the factors as follows. First we generated a random positive diagonal matrix A_{11} to form $A \in \mathcal{A}$. For N, we constructed a random $n \times n$ upper triangular matrix N_{11} with unit diagonal and set $N_{12} = N_{11}$. Finally, to form K we generated two random $n \times n$ matrices X and Y and let $C = X + iY$. We then computed the QR factorization of C and let K_{11} be the real part of Q and K_{12} be the imaginary part of Q. We tested Algorithms 2.2–2.3 on a large set of these matrices and observed a noticeable difference

TABLE 3.1
Results for the three approaches

	Tam's Algorithm	Algorithm 2.2	Algorithm 2.3
10×10 matrix with condition number 3×10^1			
$\|\bar{K}^t\bar{K} - I\|_2$	1×10^{-15}	6×10^{-16}	7×10^{-16}
$\|K_{11} - K_{22}\|_2$	9×10^{-16}	0	0
$\|K_{12} + K_{21}\|_2$	8×10^{-15}	0	0
$\|\bar{K} - K\|_2$	9×10^{-16}	4×10^{-16}	4×10^{-16}
$\|UN_{12}^t - N_{12}U^t\|_2$	3×10^{-15}	1×10^{-15}	2×10^{-15}
$\frac{\|UN_{22}^t - I\|_2}{\|U\|_2}$	0	2×10^{-16}	5×10^{-16}
$\frac{\|\bar{N} - N\|_2}{\|N\|_2}$	8×10^{-16}	5×10^{-16}	1×10^{-15}
$\frac{\|\bar{A} - A\|_2}{\|A\|}$	3×10^{-16}	2×10^{-16}	2×10^{-16}
$\frac{\|S - \bar{K}\bar{A}\bar{N}\|_2}{\|S\|_2}$	3×10^{-16}	4×10^{-16}	5×10^{-16}
100×100 matrix with condition number 7×10^4			
$\|\bar{K}^t\bar{K} - I\|_2$	1×10^{-10}	2×10^{-15}	8×10^{-14}
$\|K_{11} - K_{22}\|_2$	6×10^{-11}	0	0
$\|K_{12} + K_{21}\|_2$	6×10^{-11}	0	0
$\|\bar{K} - K\|_2$	7×10^{-11}	7×10^{-14}	8×10^{-14}
$\|UN_{12}^t - N_{12}U^t\|_2$	3×10^{-09}	2×10^{-12}	2×10^{-11}
$\frac{\|UN_{22}^t - I\|_2}{\|U\|_2}$	2×10^{-15}	7×10^{-15}	3×10^{-14}
$\frac{\|\bar{N} - N\|_2}{\|N\|_2}$	7×10^{-11}	6×10^{-12}	3×10^{-12}
$\frac{\|\bar{A} - A\|_2}{\|A\|}$	2×10^{-11}	2×10^{-15}	5×10^{-15}
$\frac{\|S - \bar{K}\bar{A}\bar{N}\|_2}{\|S\|_2}$	6×10^{-15}	1×10^{-15}	7×10^{-14}
4×4 matrix S in (3.1) with $t = 8$; condition number 10^7			
$\|\bar{K}^t\bar{K} - I\|_2$	3×10^{-03}	2×10^{-16}	2×10^{-16}
$\|K_{11} - K_{22}\|_2$	3×10^{-03}	0	0
$\|K_{12} + K_{21}\|_2$	1×10^{-03}	0	0
$\|UN_{12}^t - N_{12}U^t\|_2$	6×10^{-08}	2×10^{-10}	5×10^{-10}
$\frac{\|UN_{22}^t - I\|_2}{\|U\|_2}$	0	4×10^{-10}	1×10^{-10}
$\frac{\|S - \bar{K}\bar{A}\bar{N}\|_2}{\|S\|_2}$	2×10^{-10}	3×10^{-16}	3×10^{-16}

in the accuracy of the computed factors compared to the approach suggested in [8], even when the corrected code is used for the latter method. Algorithms 2.2–2.3 are more accurate, especially for matrices with relatively high condition numbers. In particular, the factor $\bar{K}$ may be far from being orthogonal when the method in [8] is used. Also, with that method the computed $\bar{N}$ may not satisfy the simplecticity conditions to high relative accuracy.

Table 3.1 shows some sample computational results comparing the three algorithms. The first two examples use "random" matrices constructed as described above. For those instances we compare the computed factors $\bar{K}$, $\bar{A}$ and $\bar{N}$ to the factors K, A and N used to construct the symplectic matrix S. In addition, we compute errors to measure the departure of the computed factors from satisfying the simplecticity conditions. For the last example we use the following symplectic matrix

$$S = \begin{pmatrix} \cosh t & \sinh t & 0 & \sinh t \\ \sinh t & \cosh t & \sinh t & 0 \\ 0 & 0 & \cosh t & -\sinh t \\ 0 & 0 & -\sinh t & \cosh t \end{pmatrix}, \qquad t \in \mathbb{R}. \tag{3.1}$$

For the first example, which is well conditioned, all three approaches yield good approximations to the Iwasawa factors (by any measure). When the symplectic matrix S to be factored is larger and/or has a higher condition number, as in the second example, we begin to notice some loss of (forward) accuracy in some of the factors computed using Tam's algorithm. As it may be expected, the effect is also present with the other two methods, but is less pronounced. Finally, the third example shows that accuracy can be seriously compromised when Tam's method is used. Similar trends were noticed in all our numerical experiments.

4. Implementation. For completeness, we include the MATLAB code we used to test Algorithm 2.3.

```
function [K,A,N] = iFactor(S);
%
% This function computes the Iwasawa decomposition of
% a real symplectic matrix of order 2n.
%
% Input: a real symplectic matrix [S_11  S_12; S_21  S_22]
%
% Output: K    =  2n-by-2n orthogonal symplectic matrix
%         A    =  2n-by-2n positive diagonal symplectic matrix
%         N    =  2n-by-2n "triangular" symplectic matrix
%
% s.t.
%
%         S    =  K*A*N
%

n_2   = size(S);
n     = n_2/2;

% Compute thin QR factorization of S1 = [S_11; S_21].

S_11  = S(1:n,1:n);
S_21  = S(n+1:n_2,1:n);

S1    = [S_11; S_21];
[Q,R] = qr(S1,0);

Q_11  = Q(1:n,1:n);
Q_21  = Q(n+1:n_2,1:n);

% Compute U and D from given R where U is unit upper triangular
```

```
% and H is a diagonal matrix such that R = H*U and
% R'*R = U'*H^2*U.


H     = diag(diag(R));
U     = H\R;

% Compute blocks for the factors K, A, N.

h           = sign(diag(H));
SQRT_D      = diag(h.*diag(H));
SQRT_D_inv  = diag(1./diag(SQRT_D));
h           = h';
h           = h(ones(1,n),:);
K_11        = Q_11.*h;
K_12        = -Q_21.*h;

% Form the Iwasawa factors K, A, N.

A     = [SQRT_D zeros(n) ; zeros(n) SQRT_D_inv];
K     = [K_11 K_12; -K_12 K_11];
S1    = S(1:n_2,n+1:n_2);
N1    = A\(K'*S1);
N     = [U N1(1:n,1:n); zeros(n) N1(n+1:n_2,1:n)];
```

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