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Applied Mathematics Letters 20 (2007) 260–265

Applied Mathematics Letters

www.elsevier.com/locate/aml

On the Iwasawa decomposition of a symplectic matrix

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Received 28 February 2006; received in revised form 11 April 2006; accepted 20 April 2006

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 described by T.-Y. Tam in [Computing Iwasawa decomposition of a symplectic matrix by Cholesky factorization, Appl. Math. Lett. (in press) doi:10.1016/j.aml.2006.03.001].

Keywords: Iwasawa decomposition; Symplectic group; QR factorization; Numerical stability; Cholesky factorization

1. Introduction

A matrix $S \in \mathbb{R}^{2n \times 2n}$ is called *symplectic* if it satisfies $S^t J S = J$, 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 $\mathcal{S} = Sp(n, \mathbb{R}) = \{S \in SL_{2n}(\mathbb{R}) : S^t J S = J\}$, 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 $\mathcal{S}$:

$$\mathcal{K} = \left\{ K = \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix} : K_{11} + \mathrm{i}K_{12} \in U(n) \right\} = O(2n) \cap Sp(n, \mathbb{R}),$$

$$\mathcal{A} = \left\{ \begin{pmatrix} A_{11} & 0 \\ 0 & A_{11}^{-1} \end{pmatrix} : A_{11} \text{ positive diagonal} \right\},$$

$$\mathcal{N} = \left\{ \begin{pmatrix} N_{11} & N_{12} \\ 0 & N_{11}^{-t} \end{pmatrix} : N_{11} \text{ unit upper triangular}\,,\ N_{11} N_{12}^t = N_{12} N_{11}^t \right\}.$$

The first of these three subgroups is compact, the second is abelian, and the third is nilpotent. The decomposition $\mathcal{S} = \mathcal{K}\mathcal{A}\mathcal{N}$ is called the *Iwasawa decomposition* of $\mathcal{S}$. Any $S \in Sp(n, \mathbb{R})$ can be written as $S = KAN$, where

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0893-9659/$ - see front matter
doi:10.1016/j.aml.2006.04.004

$K \in \mathcal{K}$, $A \in \mathcal{A}$, 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 a method for explicitly computing the Iwasawa decomposition $S = KAN$ of a symplectic matrix using the Cholesky factorization of $S^t S$. The approach in [8], however, does not take numerical stability considerations into account and may lead to inaccurate results in finite precision computations. It is also not very efficient in terms of operation count. Here we give a more accurate and efficient algorithm for computing the Iwasawa decomposition of a symplectic matrix.

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* $S^t S = \begin{pmatrix} A_1 & B_1 \\ B_1^t & D_1 \end{pmatrix}$ *(also in* $\mathcal{S}$*). Let* $A_1 = U^t H U$ *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*

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

is the Iwasawa decomposition of S.

On the basis of Theorem 2.1, the author of [8] proposes a Cholesky-based approach for explicitly determining the Iwasawa factors K, A, N of a given symplectic matrix. This approach has certain drawbacks. The main problem is that the approach in [8] may lead to inaccurate results in finite precision arithmetic. It is well known that forming the product $S^t S$ 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 $S^t S$ may even result in loss of positive definiteness, with the consequent breakdown of the Cholesky factorization. It is also important to avoid the use of explicit matrix inverses when computing the factorization. Although efficiency is not the primary concern of this note, it is also worth noting that the approach in [8] has a rather high computational complexity.

It is possible to 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 $S_{11} + \mathrm{i}S_{12}$; denote by U the unitary factor of $S_{11} + \mathrm{i}S_{12}$.
2. Compute the Iwasawa factors K, A and N of S as follows:

$$K_{11} = \frac{1}{2}(U + \bar{U}), \qquad K_{12} = \frac{\mathrm{i}}{2}(\bar{U} - U),$$

$$K = \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix},$$

$$\hat{N} = K^t S$$

$$A = \mathrm{diag}(\hat{n}_{11}, \ldots, \hat{n}_{2n,2n}), \text{ where } \hat{n}_{ii} \text{ are the diagonal entries of } \hat{N},$$

$$N = A^{-1}\hat{N}.$$

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 $S_1 = \binom{S_{11}}{S_{21}}$.

2. Compute the thin QR factorization of S_1, where $Q = \binom{Q_{11}}{Q_{21}}$ 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 $R_{11}^t R_{11} = U^t DU$, where $D = H^2$.
4. Compute the Iwasawa factors A, K and N of S as follows:

$$A = \begin{pmatrix} D^{\frac{1}{2}} & 0 \\ 0 & D^{-\frac{1}{2}} \end{pmatrix} \in \mathcal{A},$$

$$K_{11} = Q_{11} H D^{-\frac{1}{2}}, \qquad K_{12} = -Q_{21} H D^{-\frac{1}{2}},$$

$$K = \begin{pmatrix} K_{11} & K_{12} \\ -K_{12} & K_{11} \end{pmatrix} \in \mathcal{K},$$

$$N = \begin{pmatrix} U & N_{12} \\ 0 & N_{22} \end{pmatrix} \in \mathcal{N}, \quad \text{where } \begin{pmatrix} N_{12} \\ N_{22} \end{pmatrix} = A^{-1} K^t \begin{pmatrix} S_{12} \\ S_{22} \end{pmatrix}.$$

To see that Algorithm 2.3 computes the Iwasawa factors, first note that $A \in \mathcal{A}$. Furthermore, we need to show that $K_{11} + \mathrm{i}K_{12}$ is unitary. To this end, it suffices to verify the following two equalities:

$$K_{11}^t K_{12} = K_{12}^t K_{11}, \qquad K_{11}^t K_{11} + K_{12}^t K_{12} = I_n.$$

For the first equality it is enough to observe that $Q_{11}^t Q_{21} = Q_{21}^t Q_{11}$. Since $S \in Sp(n, \mathbb{R})$ and hence $S_{11}^t S_{21} = S_{21}^t S_{11}$, the first equation follows. The second equality can be rewritten as

$$D^{-\frac{1}{2}} U^{-t} (S_{11}^t S_{11} + S_{21}^t S_{21}) U^{-1} D^{-\frac{1}{2}} = I_n.$$

Since $S_{11}^t S_{11} + S_{21}^t S_{21} = U^t DU$ we conclude that $K_{11} + \mathrm{i}K_{12} \in U(n)$ and therefore $K \in \mathcal{K}$. It can be easily seen using the symplecticity of S that $N_{22} = U^{-t}$. Using the fact that $A_1^{-1} B_1 = B_1^t A_1^{-t}$ where A_1 and B_1 are as in Theorem 2.1 one can easily show that $UN_{12}^t = N_{12} U^t$, and hence $N \in \mathcal{N}$. Finally note that $KAN = S$.

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. This is somewhat less than the cost of the method proposed in [8], which can be shown to be $\frac{48}{3}n^3 + O(n^2)$ operations. 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 might be 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 $C = X + \mathrm{i}Y$. 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 and 2.3 on a large set of these matrices and observed a noticeable difference in the accuracy of the computed factors compared to the approach suggested in [8]. Algorithms 2.2 and 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 suggested in [8] is used. Also, with that method the computed $\bar{N}$ may not satisfy the symplecticity conditions to high relative accuracy.

Table 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}

Table 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:

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

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 method. As 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)];
```

Acknowledgements

Thanks to Daniel Kressner and Valeria Simoncini for their comments on an earlier version of this note. The work of Michele Benzi was supported in part by the National Science Foundation grant DMS-0511336.

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