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An upper J - Hessenberg reduction of a matrix through symplectic Householder transformations

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Abstract

In this paper, we introduce a reduction of a matrix to a condensed form, the upper J - Hessenberg form, via elementary symplectic Householder transformations, which are rank-one modification of the identity. Features of the reduction are highlighted and a general algorithm is derived. Then, we study different possibilities to specify the general algorithm in order to built better versions. We are led to two variants numerically more stables that we compare to JHESS algorithm. Also, some numerical experiments for comparing the different algorithms are given.

Keywords: Indefinite inner product, structure-preserving eigenproblems, symplectic Householder transformations, SR decomposition, upper J -Hessenberg form.

2000 MSC: 65F15, 65F50

1. Introduction

Let A be a $2n \times 2n$ real matrix. The SR factorization consists in writing A as a product SR , where S is symplectic and $R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}$ is such that R_{11} , R_{12} , R_{22} are upper triangular and R_{21} is strictly upper triangular [3, 4]. This decomposition plays an important role in structure-preserving methods for solving the eigenproblem of a class of structured matrices.

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More precisely, the SR decomposition can be interpreted as the analogue of the QR decomposition [5], when instead of an Euclidean space, one considers a symplectic space : a linear space, equipped with a skew-symmetric inner product (see for example [7] and the references therein). The orthogonal group with respect to this indefinite inner product, is called the symplectic group and is unbounded (contrasting with the Euclidean case).

There are two classes of methods for computing the SR decomposition. The first lies in the Gram-Schmidt like algorithms and leads to the symplectic Gram-Schmidt (SGS) algorithms. The second class is constructed from a variety of elementary symplectic transformations. Each choice of such transformations leads to the corresponding SR decomposition. Since these elementary transformations are quite heterogeneous, the SR decomposition is considerably affected by their choice.

Results on numerical aspects of SGS-algorithms can be found for example in [7]. These algorithms and their modified versions are usually involved in structure-preserving Krylov subspace-type methods, for sparse and large structured matrices.

In the literature, the symplectic elementary transformations involved in the SR decomposition can be partitioned in two subsets. The first subset is constituted of two kind of both symplectic and orthogonal transformations introduced in [6, 12] and a third symplectic but non-orthogonal transformations, proposed in [2]. In fact, in [3], it has been shown that SR decomposition of a general matrix could not be carried out by using only the above orthogonal and symplectic transformations. An algorithm, named SRDECO, based on these three transformations was derived in [2].

From linear algebra point of view, the SR decomposition via SRDECO algorithm does not correspond to the analogue of Householder QR decomposition, since SRDECO involves transformations which are not elementary rank-one modification of the identity (transvections), see [1, 5].

In [8] a study, based on linear algebra concepts and focusing on the construction of the analogue of Householder transformations in a symplectic linear space, has been accomplished. This has led to the second subset of transformations. Such analogue transformations, which are rank-one modification of the identity are called symplectic Householder transformations. Their main features have been established, especially the mapping problem has been solved. Then, the analogue of Householder QR decomposition in a symplectic linear space has been derived. The algorithm SRSR for computing the SR decomposition, using these symplectic Householder transformations

has been then presented in details. Unlike Householder QR decomposition, the new algorithm SRSH involves free parameters and advantages may be taken from this fact. It has been demonstrated how these parameters can be determined in an optimal way providing an optimal version[9] of the algorithm (SROSH). The error analysis and computational aspects of this algorithm have been studied [10]. Also, recently, a mathematical and numerical equivalence between modified symplectic Gram-Schmidt and Householder SR algorithms (typically SRSH or SROSH) have been established in [11]. Computational aspects and numerical comparisons between SGS and SROSH have clearly showed the superiority of SROSH over SGS.

In order to build a SR -algorithm (which is a QR -like algorithm) for computing the eigenvalues and eigenvectors of a matrix [13], a reduction of the matrix to an upper J -Hessenberg form is crucial. This is due to the fact that the final algorithm we are looking for should have $O(n^3)$ as complexity.

In [2], a reduction of a general matrix to an upper J -Hessenberg form is presented, using to this aim, the three symplectic transformations of the above first subset. The algorithm, called JHESS, is based on an adaptation of SRDECO.

In this paper, we focus on the reduction of a general matrix, to an upper J -Hessenberg form, using only the symplectic Householder transformations (the second subset above). We show how this reduction can be constructed. The new algorithm, which will be called JHSH algorithm, is based on an adaptation of SRSH algorithm. A variant of JHSH, named JHOSH is then obtained by taking some optimal choice of the free parameters. The JHOSH is numerically better than JHSH. However, to enforce the accuracy in the computations, we are led to derive another variant, based in replacing when possible, each symplectic non-orthogonal transformation by another one, which is symplectic and orthogonal. This gives rise to JHMSH algorithm.

In this work, we restrict ourselves to the construction of such algorithms and the study of their features. Numerical aspects of the new algorithms and new insights on JHESS algorithm (breakdowns/near-breakdowns and their prediction, different strategies of curing breakdowns/near-breakdowns, ...) are very important questions and deserve a detailed study in a devoted work. Nevertheless, we give an illustrating numerical example, showing in particular that the algorithms JHESS, JHMSH behave quite similarly.

The remainder of this paper is organized as follows. Section 2, is devoted to the necessary preliminaries. In the section 3, we introduce the method of

reducing a general matrix to an upper J -Hessenberg, based only on the use of symplectic Householder transformations, which are rank-one modification of the identity. Also, we present the different variants, motivated by numerical considerations. In the section 4, numerical experiments and comparisons between JHESS, JHMSH and JHOSH are given. We conclude in the section 5.

2. Preliminaries

Let J_{2n} (or simply J) be the $2n$ -by- $2n$ real matrix

$$J_{2n} = \begin{bmatrix} 0_n & I_n \\ -I_n & 0_n \end{bmatrix}, \quad (1)$$

where 0_n and I_n stand respectively for n -by- n null and identity matrices. The linear space \mathbb{R}^{2n} with the indefinite skew-symmetric inner product

$$(x, y)_J = x^T J y \quad (2)$$

is called symplectic. For $x, y \in \mathbb{R}^{2n}$, the orthogonality $x \perp' y$ stands for $(x, y)_J = 0$. The symplectic adjoint x^J of a vector x , is defined by

$$x^J = x^T J. \quad (3)$$

The symplectic adjoint of $M \in \mathbb{R}^{2n \times 2k}$ is defined by

$$M^J = J_{2k}^T M^T J_{2n}. \quad (4)$$

A matrix $S \in \mathbb{R}^{2n \times 2k}$ is called symplectic if

$$S^J S = I_{2k}. \quad (5)$$

The symplectic group (multiplicative group of square symplectic matrices) is denoted \mathbb{S} . A transformation T given by

$$T = I + cvv^J \text{ where } c \in \mathbb{R}, \ v \in \mathbb{R}^\nu \text{ (with } \nu \text{ even)}, \quad (6)$$

is called symplectic Householder transformation [8]. It satisfies

$$T^{-1} = T^J = I - cvv^J. \quad (7)$$

The vector v is called the direction of T .

For $x, y \in \mathbb{R}^{2n}$, there exists a symplectic Householder transformation T such that $Tx = y$ if $x = y$ or $y^J x \neq 0$. When $y^J x \neq 0$, T is given by

$$T = I + \frac{1}{y^J x}(y - x)(y - x)^J.$$

Moreover, each non null vector x can be mapped onto any non null vector y by a product of at most two symplectic Householder transformations [8]. Symplectic Householder transformations are rotations, i.e. $\det(T) = 1$ and the symplectic group \mathbb{S} is generated by symplectic Householder transformations.

We recall that a matrix $H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$, is upper J -Hessenberg when H_{11}, H_{21}, H_{22} are upper triangular and H_{12} is upper Hessenberg. H is called unreduced when H_{21} is nonsingular and the Hessenberg H_{12} is unreduced, i.e. the entries of the subdiagonal are all nonzero.

3. Upper J -Hessenberg reduction via symplectic Householder transformations

3.1. Toward the algorithm

Let $\{e_1, \dots, e_{2n}\}$ be the canonical basis of \mathbb{R}^{2n} and $a \in \mathbb{R}^{2n}$ be a given vector. We seek for symplectic Householder transformations T_1 and T_2 such that

$$T_1 a = \rho e_1, \tag{8}$$

for certain $\rho \in \mathbb{R}$ and

$$T_2 e_1 = e_1, \quad T_2 a = \mu e_1 + \nu e_{n+1}, \tag{9}$$

for certain $\mu, \nu \in \mathbb{R}$. The fact that T_2 is a symplectic isometry yields the necessary condition

$$(T_2 a)^J (T_2 e_1) = a^J e_1, \tag{10}$$

which implies $\nu = a_{n+1}$ (the $n+1$ th component of a) and μ is arbitrary. We get

Theorem 1. *Let $\rho \neq 0$, μ be arbitrary scalars and $\nu = a_{n+1}$. Setting*

$$c_1 = -\frac{1}{\rho a^J e_1}, \quad v_1 = \rho e_1 - a, \quad c_2 = -\frac{1}{a^J (\mu e_1 + \nu e_{n+1})}, \quad v_2 = \mu e_1 + \nu e_{n+1} - a,$$

then

$$T_1 = I + c_1 v_1 v_1^J \text{ (respectively } T_2 = I + c_2 v_2 v_2^J \text{) satisfy (8) (respectively (9)).} \quad (11)$$

Remark 1. Since the $n + 1$ th component of v_2 is zero, T_2 keeps the $n + 1$ th component of $T_2 x$ unchanged, for any $x \in \mathbb{R}^{2n}$. More on the properties of such transformations T_1 or T_2 can be found in [9, 10].

We also need the following

Theorem 2. Let $v \in \mathbb{R}^{2n}$, with the partition $v = [0^T, u^T, 0^T, w^T]^T$, where $[u, w] \in \mathbb{R}^{(n-i) \times 2}$, for a given integer $1 \leq i \leq n - 1$ and set $\tilde{v} = [u^T, w^T]^T$. Consider the symplectic transformations $T = I + cvv^J$ and $\tilde{T} = I + c\tilde{v}\tilde{v}^J$. We have

$$\forall \alpha \in \mathbb{R}^i, \forall \beta \in \mathbb{R}^i, \forall x \in \mathbb{R}^{n-i}, \forall y \in \mathbb{R}^{n-i},$$

$$T[\alpha^T, x^T, \beta^T, y^T]^T = [\alpha^T, x'^T, \beta^T, y'^T]^T, \text{ with } [x'^T, y'^T]^T = \tilde{T}[x^T, y^T]^T.$$

PROOF. We have $v^J[\alpha^T, x^T, \beta^T, y^T]^T = u^T y - w^T x = [u^T w^T] J [x^T y^T]^T$. Then $T[\alpha^T, x^T, \beta^T, y^T]^T = [\alpha^T, x^T, \beta^T, y^T]^T + c[0^T, u^T, 0^T, w^T]^T [u^T w^T] J [x^T y^T]^T$. We check easily $\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix} + c \begin{bmatrix} u \\ w \end{bmatrix} [u^T w^T] J \begin{bmatrix} x \\ y \end{bmatrix} = \tilde{T} \begin{bmatrix} x \\ y \end{bmatrix}$, and $T[\alpha^T, 0^T, \beta^T, 0^T]^T = [\alpha^T, 0^T, \beta^T, 0^T]^T$.

Note that the Theorem 2 remains valid if one takes T^J instead of T . This result, with Theorem 1, constitute the main tool on which the *SR* factorization (based on symplectic Householder transformations) is constructed. We will adapt this tool for reducing a general matrix to an upper *J*-Hessenberg form, based on these symplectic Householder transformations.

3.2. The *J*-Hessenberg reduction : the *JHSH* algorithm

We explain here the steps of the algorithm by illustrating the general pattern. Let $A \in \mathbb{R}^{2n \times 2n}$ be a given matrix and set $A^{(0)} = A$. We will use the notation $A_{(i_1:i_2, j_1:j_2)}$, $A_{(i_1:i_2, :)}$, $A_{(:, j_1:j_2)}$ to denote respectively the submatrix obtained from the matrix A by deleting all rows and columns except rows i_1 until i_2 and columns j_1 until j_2 , by deleting all rows except rows i_1 until i_2 , by deleting all columns except columns j_1 until j_2 .

1. The first step of the algorithm relies in determining a symplectic Householder transformation H_1 (i.e. $c_1 \in \mathbb{R}$ and $v_1 \in \mathbb{R}^{2n}$), with $H_1 e_1 = e_1$, to zero

out entries 2 through n and entries $n + 2$ through $2n$ of the first column of $A^{(0)}$. The vector e_1 stands for the first canonical vector of \mathbb{R}^{2n} . The transformation H_1 corresponds to the transformation T_2 , given in Theorem 1. Set v_1 the direction vector of H_1 . Since $H_1 e_1 = e_1$, we obtain $v_1^J e_1 = v_1^T J e_1 = 0$. Thus the $n + 1$ th component of v_1 is zero. It follows that for any vector x , the $n + 1$ th component of $H_1 x$ remains unchanged. The direction v_1 of H_1 is given by $v_1 = A_{(1,1)}^{(1)} e_1 + A_{(n+1,1)}^{(0)} e_{n+1} - A_{(:,1)}^{(0)}$, where $A_{(1,1)}^{(1)}$ is an arbitrary given scalar. Notice that we have also $H_1^J e_1 = e_1$, and hence the first column of H_1 and H_1^J is e_1 . Thus, multiplying $A^{(0)}$ on the left by H_1 leaves unchanged the $n + 1$ th row and creates the desired zeros in the first column. We get

$$A'^{(1)} = H_1 A^{(0)} = \begin{bmatrix} A_{(1,1)}^{(1)} & A'_{(1,2:n)}^{(1)} & A'_{(1,n+1:2n)}^{(1)} \\ 0 & A_{(2:n,2:n)}^{(1)} & A_{(2:n,n+1:2n)}^{(1)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2:n)}^{(0)} & A_{(n+1,n+1:2n)}^{(0)} \\ 0 & A_{(n+2:2n,2:n)}^{(1)} & A_{(n+2:2n,n+1:2n)}^{(1)} \end{bmatrix}.$$

The step involves the free parameter $A_{(1,1)}^{(1)}$.

Multiplying $H_1 A^{(0)}$ on the right by H_1^J leaves the first column of $H_1 A^{(0)} H_1^J$ unchanged, and we obtain

$$A^{(1)} = H_1 A^{(0)} H_1^J = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2:n)}^{(1)} & A_{(1,n+1:2n)}^{(1)} \\ 0 & A_{(2:n,2:n)}^{(1)} & A_{(2:n,n+1:2n)}^{(1)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2:n)}^{(1)} & A_{(n+1,n+1:2n)}^{(1)} \\ 0 & A_{(n+2:2n,2:n)}^{(1)} & A_{(n+2:2n,n+1:2n)}^{(1)} \end{bmatrix}.$$

The next step consists in choosing a symplectic Householder H_2 to zero out the entries 3 through n , the entries $n + 2$ through $2n$ of the $n + 1$ th column of $A^{(1)}$. To do this, let $\tilde{A}^{(1)} = \begin{bmatrix} A_{(2:n,2:n)}^{(1)} & A_{(2:n,n+1:2n)}^{(1)} \\ A_{(n+2:2n,2:n)}^{(1)} & A_{(n+2:2n,n+1:2n)}^{(1)} \end{bmatrix}$ be the matrix obtained from $A^{(1)}$ by deleting the first column and the first and the $n + 1$ th rows. And let $A_{(2,n+1)}^{(2)} \neq 0$ be an arbitrary given scalar.

We apply $\tilde{H}_2 = I_{2n-2} + c_2 \tilde{v}_2 \tilde{v}_2^J$ given by Theorem 1, with $\tilde{v}_2 = \begin{bmatrix} u_2 \\ w_2 \end{bmatrix} = A_{(2,n+1)}^{(2)} e_1 - \tilde{A}^{(1)}(:, n) \in \mathbb{R}^{2n-2}$, $u_2 \in \mathbb{R}^{n-1}$, $w_2 \in \mathbb{R}^{n-1}$, where e_1 stands for

the first canonical vector of \mathbb{R}^{2n-2} . We obtain

$$\tilde{A}'^{(2)} = \tilde{H}_2 \tilde{A}^{(1)} = \begin{bmatrix} A_{(2,2:n)}^{(2)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2:2n)}^{(2)} \\ A_{(3:n,2:n)}^{(2)} & 0 & A_{(3:n,n+2:2n)}^{(2)} \\ A_{(n+2:2n,2:n)}^{(2)} & 0 & A_{(n+2:2n,n+2:2n)}^{(2)} \end{bmatrix}.$$

The transformation \tilde{H}_2 corresponds to the choice T_1 in Theorem 1. Setting

$$H_2 = I_{2n} + c_2 v_2 v_2^J, \text{ with } v_2 = \begin{bmatrix} 0 \\ u_2 \\ 0 \\ w_2 \end{bmatrix} \in \mathbb{R}^{2n} \text{ then } H_2 \text{ is a symplectic}$$

Householder transformation. Using Theorem 2, we get

$$A'^{(2)} = H_2 A^{(1)} = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2:n)}^{(1)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2:2n)}^{(1)} \\ 0 & A_{(2,2:n)}^{(2)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2:2n)}^{(2)} \\ 0 & A_{(3:n,2:n)}^{(2)} & 0 & A_{(3:n,n+2:2n)}^{(2)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2:n)}^{(1)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2:2n)}^{(1)} \\ 0 & A_{(n+2:2n,2:n)}^{(2)} & 0 & A_{(n+2:2n,n+2:2n)}^{(2)} \end{bmatrix}.$$

H_2 leaves the first and the $n+1$ th rows of $H_2 A^{(1)}$ unchanged. It leaves the first column of $H_2 A^{(1)}$ unchanged, and creates the desired zeros in the column $n+1$.

The multiplication of $H_2 A^{(1)}$ on the right by H_2^J leaves the first and the $n+1$ th columns of $H_2 A^{(1)} H_2^J$ unchanged. We obtain

$$A^{(2)} = H_2 A^{(1)} H_2^J = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2:n)}^{(2)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2:2n)}^{(2)} \\ 0 & A_{(2,2:n)}^{(2)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2:2n)}^{(2)} \\ 0 & A_{(3:n,2:n)}^{(2)} & 0 & A_{(3:n,n+2:2n)}^{(2)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2:n)}^{(2)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2:2n)}^{(2)} \\ 0 & A_{(n+2:2n,2:n)}^{(2)} & 0 & A_{(n+2:2n,n+2:2n)}^{(2)} \end{bmatrix}.$$

It is worth noting that $H_2 e_1 = e_1$ and $H_2 e_{n+1} = e_{n+1}$. Thus the first column (respectively the $n+1$ th column) of H_2 and H_2^J is e_1 (respectively e_{n+1}).

In the next step, we want to zero out the entries 3 through n and $n+3$ through $2n$ of the second column of $A^{(2)}$ and the entries 4 through n and $n+3$ through $2n$ of the column $n+2$ of $A^{(2)}$. Let $\tilde{A}^{(2)}$ be the matrix obtained from

$A^{(2)}$ by deleting the first, the $n + 1$ th rows, and the corresponding columns,

$$\text{ie. } \tilde{A}^{(2)} = \begin{bmatrix} A_{(2:n,2:n)}^{(2)} & A_{(2:n,n+2:2n)}^{(2)} \\ A_{(n+2:2n,2:n)}^{(2)} & A_{(n+2:2n,n+2:2n)}^{(2)} \end{bmatrix}.$$

2. We apply now exactly the same two steps of **1.**, to the new size reduced matrix $\tilde{A}^{(2)}$. In other words, we choose a symplectic Householder transformation \tilde{H}_3 , which means to compute a vector $\tilde{v}_3 = [u_3^T, w_3^T]^T$ with $u_3 \in \mathbb{R}^{n-1}$, $w_3 \in \mathbb{R}^{n-1}$ and a real c_3 such that $\tilde{H}_3 = I + c_3 \tilde{v}_3 \tilde{v}_3^J$ zero out the entries 2 through $n - 1$ and the entries $n + 1$ through $2n - 2$ of the first column of $\tilde{A}^{(2)}$ with $\tilde{H}_3 e_1 = e_1 \in \mathbb{R}^{2n-2}$. Here e_1 stands for the first canonical vector of \mathbb{R}^{2n-2} . The transformation \tilde{H}_3 corresponds to the transformation T_2 , in Theorem 1. Let e_n denote the n th canonical vector of \mathbb{R}^{2n-2} . The direction vector \tilde{v}_3 of \tilde{H}_3 is given by $\tilde{v}_3 = A_{(2,2)}^{(3)} e_1 + \tilde{A}^{(2)}(n, 1) e_n - \tilde{A}^{(2)}(:, 1)$, where $A_{(2,2)}^{(3)}$ is an arbitrary non zero scalar. \tilde{H}_3 leaves unchanged the n th row of $\tilde{H}_3 \tilde{A}^{(2)}$. We get

$$\tilde{A}'^{(3)} = \tilde{H}_3 \tilde{A}^{(2)} = \begin{bmatrix} A_{(2,2)}^{(3)} & A_{(2,3:n)}'^{(3)} & A_{(2,n+2:2n)}'^{(3)} \\ 0 & A_{(3:n,3:n)}'^{(3)} & A_{(3:n,n+2:2n)}'^{(3)} \\ A_{(n+2,2)}^{(2)} & A_{(n+2,3:n)}^{(2)} & A_{(n+2,n+2:2n)}^{(2)} \\ 0 & A_{(n+3:2n,3:n)}'^{(3)} & A_{(n+3:2n,n+2:2n)}'^{(3)} \end{bmatrix}.$$

Remark that the n th component of \tilde{v}_3 is zero. Take now $v_3 = [0 \ u_3^T \mid 0 \ w_3^T]^T$ and set $H_3 = I + c_3 v_3 v_3^J$. Then H_3 is obviously a symplectic Householder transformation of order $2n$. The components 1, $n + 1$ and $n + 2$ of v_3 are equal to zero. Thus H_3 leaves the rows 1, $n + 1$ and $n + 2$ of $H_3 A^{(2)}$ unchanged and satisfy $H_3(e_1) = e_1$, $H_3 e_2 = e_2$ and $H_3 e_{n+1} = e_{n+1}$. Thus H_3 leaves the first and the $n + 1$ th columns of $H_3 A^{(2)}$ unchanged and zero out the entries 3 through n and the entries $n + 3$ through $2n$ of the second column.

We have

$$A'^{(3)} = H_3 A^{(2)} = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2)}^{(2)} & A_{(1,3:n)}^{(2)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2:2n)}^{(2)} \\ 0 & A_{(2,2)}^{(3)} & A_{(2,3:n)}'^{(3)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2:2n)}'^{(3)} \\ 0 & 0 & A_{(3:n,3:n)}'^{(3)} & 0 & A_{(3:n,n+2:2n)}'^{(3)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2)}^{(2)} & A_{(n+1,3:n)}^{(2)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2:2n)}^{(2)} \\ 0 & A_{(n+2,2)}^{(2)} & A_{(n+2,3:n)}^{(2)} & 0 & A_{(n+2,n+2:2n)}^{(2)} \\ 0 & 0 & A_{(n+3:2n,3:n)}'^{(3)} & 0 & A_{(n+3:2n,n+2:2n)}'^{(3)} \end{bmatrix}.$$

The transformation H_3^J leaves the column 1, 2 and $n+1$ of $H_3 A^{(2)} H_3^J$ unchanged since $H_3^J(e_1) = e_1$, $H_3^J e_2 = e_2$ and $H_3^J e_{n+1} = e_{n+1}$. We get

$$A^{(3)} = H_3 A^{(2)} H_3^J = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2)}^{(2)} & A_{(1,3:n)}^{(3)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2:2n)}^{(3)} \\ 0 & A_{(2,2)}^{(3)} & A_{(2,3:n)}^{(3)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2:2n)}^{(3)} \\ 0 & 0 & A_{(3:n,3:n)}^{(3)} & 0 & A_{(3:n,n+2:2n)}^{(3)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2)}^{(2)} & A_{(n+1,3:n)}^{(3)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2:2n)}^{(3)} \\ 0 & A_{(n+2,2)}^{(2)} & A_{(n+2,3:n)}^{(3)} & 0 & A_{(n+2,n+2:2n)}^{(3)} \\ 0 & 0 & A_{(n+3:2n,3:n)}^{(3)} & 0 & A_{(n+3:2n,n+2:2n)}^{(3)} \end{bmatrix}.$$

Now, deleting the rows 1, 2, $n+1$, $n+2$ and the columns 1, 2, $n+1$ of $A^{(3)}$ and setting $\tilde{A}^{(3)} = \begin{bmatrix} A_{(3:n,3:n)}^{(3)} & A_{(3:n,n+2:2n)}^{(3)} \\ A_{(n+3:2n,3:n)}^{(3)} & A_{(n+3:2n,n+2:2n)}^{(3)} \end{bmatrix}$, we find $c_4 \in \mathbb{R}$ and $\tilde{v}_4 = \begin{bmatrix} u_4 \\ w_4 \end{bmatrix}$, with $u_4 \in \mathbb{R}^{n-2}$ and $w_4 \in \mathbb{R}^{n-2}$ such that the action of $\tilde{H}_4 = I + c_4 \tilde{v}_4 \tilde{v}_4^J$ gives

$$\tilde{A}'^{(4)} = \tilde{H}_4 \tilde{A}^{(3)} = \begin{bmatrix} A_{(3,3:n)}'^{(4)} & A_{(3,n+2)}^{(4)} & A_{(3,n+3:2n)}'^{(4)} \\ A_{(4:n,3:n)}'^{(4)} & 0 & A_{(4:n,n+3:2n)}'^{(4)} \\ A_{(n+3:2n,3:n)}'^{(4)} & 0 & A_{(n+3:2n,n+3:2n)}'^{(4)} \end{bmatrix}.$$

The coefficient $A_{(3,n+2)}^{(4)}$ is an arbitrary chosen scalar. Taking $v_4 = [0 \ 0 \ u_4^T | 0 \ 0 \ w_4^T]^T$ then the transformation $H_4 = I + c_4 v_4 v_4^J$ leaves unchanged the rows 1, 2, $n+1$, $n+2$ and columns 1, 2, and $n+1$ of $A'^{(4)} = H_4 A^{(3)}$ and creates the desired zeros in the column $n+2$. We obtain

$$A'^{(4)} = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2)}^{(2)} & A_{(1,3:n)}^{(3)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2)}^{(3)} & A_{(1,n+3:2n)}^{(3)} \\ 0 & A_{(2,2)}^{(3)} & A_{(2,3:n)}^{(3)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2)}^{(3)} & A_{(2,n+3:2n)}^{(3)} \\ 0 & 0 & A_{(3,3:n)}'^{(4)} & 0 & A_{(3,n+2)}^{(4)} & A_{(3,n+3:2n)}'^{(4)} \\ 0 & 0 & A_{(4:n,3:n)}'^{(4)} & 0 & 0 & A_{(4:n,n+3:2n)}'^{(4)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2)}^{(2)} & A_{(n+1,3:n)}^{(3)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2)}^{(3)} & A_{(n+1,n+3:2n)}^{(3)} \\ 0 & A_{(n+2,2)}^{(2)} & A_{(n+2,3:n)}^{(3)} & 0 & A_{(n+2,n+2)}^{(3)} & A_{(n+2,n+3:2n)}^{(3)} \\ 0 & 0 & A_{(n+3:2n,3:n)}'^{(4)} & 0 & 0 & A_{(n+3:2n,n+3:2n)}'^{(4)} \end{bmatrix}.$$

H_4^J leaves unchanged the first, the second, the $n+1$, $n+2$ columns of $A^{(4)} = H_4 A^{(3)} H_4^J$ since $H_4^J(e_i) = e_i$ for $i = 1, 2, n+1, n+2$. Hence, we get

$$A^{(4)} = \begin{bmatrix} A_{(1,1)}^{(1)} & A_{(1,2)}^{(2)} & A_{(1,3:n)}^{(4)} & A_{(1,n+1)}^{(1)} & A_{(1,n+2)}^{(3)} & A_{(1,n+3:2n)}^{(4)} \\ 0 & A_{(2,2)}^{(3)} & A_{(2,3:n)}^{(4)} & A_{(2,n+1)}^{(2)} & A_{(2,n+2)}^{(3)} & A_{(2,n+3:2n)}^{(4)} \\ 0 & 0 & A_{(3,3:n)}^{(4)} & 0 & A_{(3,n+2)}^{(4)} & A_{(3,n+3:2n)}^{(4)} \\ 0 & 0 & A_{(4:n,3:n)}^{(4)} & 0 & 0 & A_{(4:n,n+3:2n)}^{(4)} \\ A_{(n+1,1)}^{(0)} & A_{(n+1,2)}^{(2)} & A_{(n+1,3:n)}^{(4)} & A_{(n+1,n+1)}^{(1)} & A_{(n+1,n+2)}^{(3)} & A_{(n+1,n+3:2n)}^{(4)} \\ 0 & A_{(n+2,2)}^{(2)} & A_{(n+2,3:n)}^{(4)} & 0 & A_{(n+2,n+2)}^{(3)} & A_{(n+2,n+3:2n)}^{(4)} \\ 0 & 0 & A_{(n+3:2n,3:n)}^{(4)} & 0 & 0 & A_{(n+3:2n,n+3:2n)}^{(4)} \end{bmatrix}.$$

3. The j th step is now clear. It involves two sub-steps. The first consists in finding H_{2j-1} , i.e. the scalar c_{2j-1} and the vector v_{2j-1} such that $H_{2j-1} = I + c_{2j-1} v_{2j-1} v_{2j-1}^J$ leaves the rows $1, \dots, j-1$, the rows $n+1, \dots, n+j$, the columns $1, \dots, j-1$, and the columns $n+1, \dots, n+j-1$ of $H_{2j-1} A^{(2j-2)}$ unchanged and zero out the entries $j+1$ through n and the entries $n+j+1$ through $2n$ of the j th column. The vector $v_{2j-1} \in \mathbb{R}^{2n}$ has the structure $v_{2j-1} = [0^T, u_{2j-1}^T, 0^T, w_{2j-1}^T]^T$, with $u_{2j-1} \in \mathbb{R}^{n-j+1}$, $w_{2j-1} \in \mathbb{R}^{n-j+1}$. The first component of w_{2j-1} is zero. Thus $H_{2j-1} e_i = e_i$ for $i = 1, \dots, j$ and for $i = n+1, \dots, n+j-1$. The j th column $H_{2j-1} A^{(2j-2)}(:, j)$ is transformed as follows

$$H_{2j-1} A^{(2j-2)}(:, j) = \begin{bmatrix} A^{(2j-2)}(1:j-1, j) \\ A^{(2j-1)}(j, j) \\ 0 \\ A^{(2j-2)}(n+1:n+j, j) \\ 0 \end{bmatrix} \begin{matrix} \{j-1\} \\ \{1\} \\ \{n-j\} \\ \{j\} \\ \{n-j\} \end{matrix}.$$

The entry $A^{(2j-1)}(j, j)$ is a free parameter.

The multiplication of $H_{2j-1} A^{(2j-2)}$ on the right by H_{2j-1}^J leaves the columns $1, \dots, j$, and the columns $n+1, \dots, n+j-1$, of $H_{2j-1} A^{(2j-2)} H_{2j-1}^J$ unchanged. The coefficient c_{2j-1} , the vector v_{2j-1} and hence the symplectic transformation H_{2j-1} are simply and explicitly given by Theorem 1. The matrix $A^{(2j-1)} = H_{2j-1} A^{(2j-2)} H_{2j-1}^J$ has the desired form. Let us set $\tilde{H}_{2j-1} = I + c_{2j-1} \tilde{v}_{2j-1} \tilde{v}_{2j-1}^J$, $\tilde{v}_{2j-1} = [u_{2j-1}^T, w_{2j-1}^T]^T$, where $[u_{2j-1}, w_{2j-1}] \in \mathbb{R}^{\alpha_j \times 2}$, with $\alpha_j = n-j+1$ and $\tilde{A}^{(2j-2)}(:, j)$ the j th column of $\tilde{A}^{(2j-2)}$ obtained from $A^{(2j-2)}(:, j)$ by deleting the rows $1, \dots, j-1$ and rows $n+1, \dots, n+j-1$. We

obviously obtain $\tilde{H}_{2j-1}\tilde{A}^{(2j-2)}(:, j) = A^{(2j-1)}(j, j)e_1 + A^{(2j-2)}(n+j, j)e_{\alpha_j+1}$. Here e_1 and e_{α_j+1} denote the first and the α_j+1 th canonical vectors of $\mathbb{R}^{2\alpha_j}$.

In a similar way, the second sub-step consists in finding H_{2j} , i.e. the scalar c_{2j} and the vector v_{2j} such that $H_{2j} = I + c_{2j}v_{2j}v_{2j}^J$ leaves the rows $1, \dots, j$, the rows $n+1, \dots, n+j$, the columns $1, \dots, j$, and the columns $n+1, \dots, n+j-1$ of $H_{2j}A^{(2j-1)}$ unchanged and zero out the entries $j+2$ through n and the entries $n+j+1$ through $2n$ of the $n+j$ th column. The vector $v_{2j} \in \mathbb{R}^{2n}$ has the structure $v_{2j} = [0^T, u_{2j}^T, 0^T, w_{2j}^T]^T$, with $u_{2j} \in \mathbb{R}^{n-j}$, $w_{2j} \in \mathbb{R}^{n-j}$. Thus $H_{2j}e_i = e_i$ for $i = 1, \dots, j$ and for $i = n+1, \dots, n+j$. The $n+j$ th column of $H_{2j}A^{(2j-1)}(:, n+j)$ is transformed as follows

$$H_{2j}A^{(2j-1)}(:, n+j) = \begin{bmatrix} A^{(2j-1)}(1:j, n+j) \\ A^{(2j)}(j+1, n+j) \\ 0 \\ A^{(2j-1)}(n+1:n+j, n+j) \\ 0 \end{bmatrix} \begin{matrix} \{j\} \\ \{1\} \\ \{n-j-1\} \\ \{j\} \\ \{n-j\} \end{matrix}.$$

The entry $A^{(2j)}(j+1, n+j)$ is a free parameter.

The multiplication of $H_{2j}A^{(2j-1)}$ on the right by H_{2j}^J leaves the columns $1, \dots, j$, and the columns $n+1, \dots, n+j$, of $H_{2j}A^{(2j-1)}H_{2j}^J$ unchanged. The coefficient c_{2j} , the vector v_{2j} and hence the symplectic transformation H_{2j} are explicitly given by Theorem 1. The matrix $A^{(2j)} = H_{2j}A^{(2j-1)}H_{2j}^J$ has the desired form.

Let us set $\tilde{H}_{2j} = I + c_{2j}\tilde{v}_{2j}\tilde{v}_{2j}^J$, with $\tilde{v}_{2j} = [u_{2j}^T, w_{2j}^T]^T$, where $[u_{2j}, w_{2j}] \in \mathbb{R}^{\beta_j \times 2}$, $\beta_j = n-j$ and $\tilde{A}^{(2j-1)}(:, n+j)$ the $n+j$ th column of $\tilde{A}^{(2j-1)}$ obtained from $A^{(2j-1)}(:, n+j)$ by deleting the rows $1, \dots, j$ and rows $n+1, \dots, n+j$. We obviously obtain $\tilde{H}_{2j}\tilde{A}^{(2j-1)}(:, n+j) = A^{(2j)}(j+1, n+j)e_1$. Here e_1 denotes the first canonical vector of $\mathbb{R}^{2\beta_j}$.

Thus, it is worth noting that each step j involves two free parameters $A^{(2j-1)}(j, j)$ and $A^{(2j)}(j+1, n+j)$, and that these parameters are located as highlighted above, in the corresponding symplectic Householder transformations H_{2j-1} and H_{2j} (or equivalently \tilde{H}_{2j-1} and \tilde{H}_{2j}).

At the last step (the $n-1$ th step), we obtain

$H_{2n-2} \dots H_2 H_1 A (H_{2n-2} \dots H_2 H_1)^J = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = H \in \mathbb{R}^{2n \times 2n}$, with H_{11} , H_{21} , H_{22} upper triangular and H_{12} upper Hessenberg. We get $A = S^J H S$ with $S = H_{2n-2} \dots H_1$. The entries of the diagonal of H_{11} are the free parameters $A^{(2j-1)}(j, j)$, ie. $H_{11}(j, j) = A^{(2j-1)}(j, j)$ for $j = 1, \dots, n$. Also,

The entries of the sub-diagonal of H_{12} are the free parameters $A^{(2j)}(j+1, n+j)$, ie. $H_{12}(j+1, j) = A^{(2j)}(j+1, n+j)$ for $j = 1, \dots, n-1$. We propose here the algorithm in its general version, written in pseudo Matlab code, for computing the reduction of a matrix to the upper J -Hessenberg form, via symplectic Householder transformations (JHSH algorithm).

Algorithm 3. *function* $[S, H] = \text{JHSH}(A)$

```

    twon = size(A(:, 1)); n = twon/2; S = eye(twon);
    for j = 1 : n - 1
        J = [zeros(n - j + 1), eye(n - j + 1); -eye(n - j + 1), zeros(n - j + 1)];
        ro = [j : n, n + j : 2n]; co = [j : n, n + j : 2n];
        [c, v] = sh2(A(ro, j));
        % Updating A :
        A(ro, co) = A(ro, co) + c * v * (v' * J * A(ro, co));
        A(:, co) = A(:, co) - (A(:, co) * (c * v)) * v' * J;
        % Updating S (if needed):
        S(ro, 2 : end) = S(ro, 2 : end) + c * (v * v') * J * S(ro, 2 : end);
        J = [zeros(n - j), eye(n - j); -eye(n - j), zeros(n - j)];
        ro = [j + 1 : n, n + j + 1 : 2n];
        [c, v] = sh1(A(ro, n + j));
        %Updating A:
        A(ro, co) = A(ro, co) + c * v * (v' * J * A(ro, co));
        A(:, ro) = A(:, ro) - (A(:, ro) * (c * v)) * v' * J;
        %Updating S (if needed):
        S(ro, 2 : end) = S(ro, 2 : end) + c * (v * v') * J * S(ro, 2 : end);
    end
end

```

Algorithm 4. *function* $[c, v] = \text{sh1}(a)$

```

    %compute c and v such that  $T_1 a = \rho e_1$ ,
    %  $a = [a_1, \dots, a_{2n}]$ .
    %  $\rho$  is a free parameter, and  $T_1 = (\text{eye}(twon) + c * v * v' * J)$ ;
    twon = length(a); n = twon/2;
    J = [zeros(n), eye(n); -eye(n), zeros(n)];
    choose  $\rho$ ; aux =  $a_1 - \rho$ ;
    if aux == 0
        c = 0; v = zeros(twon, 1); %T = eye(twon);
    end

```

```

elseif  $a_{n+1} == 0$ 
display('division by zero');
return
else
 $v = \frac{a}{aux}$ ;  $c = \frac{aux^2}{\rho \times a_{n+1}}$ ;  $v(1) = 1$ ;
end
end

```

Algorithm 5. *function $[c, v] = sh2(a)$*

```

%compute c and v such that  $T_2 e_1 = e_1$ , and  $T_2 a = \mu e_1 + \nu e_{n+1}$ ,
% $\mu$  is a free parameter, and  $T_2 = (eye(twon) + c * v * v' * J)$ ;
%  $a = [a_1, \dots, a_{2n}]$ .
twon = length(a);  $n = twon/2$ ;
 $J = [zeros(n), eye(n); -eye(n), zeros(n)]$ ;
if  $n == 1$ 
 $v = zeros(twon, 1)$ ;  $c = 0$ ; % $T = eye(twon)$ ;
else
choose  $\mu$ ;
 $\nu = a_{n+1}$ ;
if  $\nu == 0$ 
display('division by zero')
return
else
 $v = \mu e_1 + \nu e_{n+1} - a$ ,  $c = \frac{1}{a_{n+1}(\mu - a_1)}$ ;
end
end

```

3.3. JHOSH, JHMSH algorithms

From an linear algebra point of view, JHSH is the analogue in the symplectic case, of the algorithm performing the Hessenberg reduction of a matrix via Householder transformations in the Euclidean case. Recall that JHSH involves two free parameters at each step. The question is then how these free parameters can be chosen? In the sequel, we show how one can take benefit from these free parameters in some optimal way. In order to get an algorithm numerically stable as possible, the free parameters are chosen so that the symplectic Householder transformations used in the reduction

have minimal norm-2 condition number. The choice of such parameters is as follows [9] :

Theorem 6. *Let $a = [a_1, \dots, a_{2n}] \in \mathbb{R}^{2n}$ be a given vector and $\{e_1, \dots, e_{2n}\}$ be the canonical basis of \mathbb{R}^{2n} . Take $\rho = \text{sign}(a_1) \|a\|_2$, $\mu = a_1 \pm \xi$ and*

$$\nu = a_{n+1}, \text{ with } \xi = \sqrt{\sum_{i=2, i \neq n+1}^{2n} a_i^2}. \text{ Setting}$$

$$c_1 = -\frac{1}{\rho a^J e_1}, \quad v_1 = \rho e_1 - a, \quad c_2 = -\frac{1}{a^J (\mu e_1 + \nu e_{n+1})}, \quad v_2 = \mu e_1 + \nu e_{n+1} - a,$$

then

$$T_1 = I + c_1 v_1 v_1^J \quad (\text{respectively } T_2 = I + c_2 v_2 v_2^J) \text{ satisfy (8) (respectively (9))}, \quad (12)$$

with T_1 (respectively T_2) has the minimal norm-2 condition number.

PROOF. See [9], Lemma 4.1, Lemma 4.3, Lemma 4.4 and Theorem 4.5.

For these choices of the free parameters, we refer to T_1 (respectively T_2) as the first optimal symplectic Householder (osh1) transformation (respectively the second optimal symplectic Householder osh2) transformation. This optimal version of JHSH is referred to as JHOSH algorithm and is given as follows :

Algorithm 7. *function $[S, H] = \text{JHOSH}(A)$*

replace in the body of JHSH the sh1 by osh1 and sh2 by osh2.
end.

The pseudo code Matlab of *osh1* and *osh2* is as follows

Algorithm 8. *function $[c, v] = \text{osh1}(a)$*

twon = length(a); n = twon/2;
J = [zeros(n), eye(n); -eye(n), zeros(n)];
 *$\rho = \text{sign}(a(1)) * \|a\|_2$; aux = a(1) - ρ ;*
if aux == 0
c = 0; v = zeros(twon, 1); %T = eye(twon);
elseif $a_{n+1} == 0$
display('division by zero');
return


```

else

$$v = \frac{a}{aux}; c = \frac{aux^2}{\rho * a_{n+1}}; v(1) = 1;$$

%T = (eye(twon) + c * v * v' * J);
end
end

```

Algorithm 9. *function [c, v] = osh2(a)*

```

twon = length(u); n = twon/2;
J = [zeros(n), eye(n); -eye(n), zeros(n)];
if n == 1
v = zeros(twon, 1); c = 0; %T = eye(twon);
else
I = [2 : n, n + 2 : twon];  $\xi = \text{norm}(a(I))$ ;
if  $\xi == 0$ 
v = zeros(twon, 1); c = 0; %T = eye(twon);
else
 $\nu = a_{n+1}$ ;
if  $\nu == 0$ 
display('division by zero')
return
else
 $v = -a/\xi$ ;  $v(1) = 1$ ;  $v(n + 1) = 0$ ;  $c = \xi/\nu$ ;
%T = (eye(twon) + c * v * v' * J);
end
end
end
end

```

We have seen that the symplectic Householder transformations used in JHOSH algorithm have minimal norm-2 condition number, and thus numerically, JHOSH presents a significant advantage over JHSH. However, all these symplectic Householder transformations are not orthogonal. It is well known that it is not possible to handle a SR decomposition using only transformations which are both symplectic and orthogonal (see [3]). Nevertheless, we will show that half of them (all the transformations H_{2j} above) may be replaced by specified transformations which are both orthogonal and symplectic. Furthermore, we will show that the two type of orthogonal and

symplectic transformations, introduced by Paige et al. [6, 12] can be used to replace the symplectic transformations H_{2j} , to zero desired components of a vector. The first type is

$$H(k, w) = \begin{pmatrix} \text{diag}(I_{k-1}, P) & 0 \\ 0 & \text{diag}(I_{k-1}, P) \end{pmatrix}, \quad (13)$$

where

$$P = I - 2ww^T/w^Tw, \quad w \in \mathbb{R}^{n-k+1}.$$

The transformation $H(k, w)$ is just a direct sum of two "ordinary" n -by- n Householder matrices [14]. We refer to $H(k, w)$ as Van Loan's Householder transformations. The second type is

$$J(k, c, s) = \begin{pmatrix} C & S \\ -S & C \end{pmatrix}, \quad (14)$$

where $c^2 + s^2 = 1$, and

$$C = \text{diag}(I_{k-1}, c, I_{n-k}),$$

$$S = \text{diag}(0_{k-1}, s, 0_{n-k}).$$

$J(k, c, s)$ is a Givens transformation, which is an "ordinary" $2n$ -by- $2n$ Givens rotation that rotates in planes $(k, k+n)$ [14]. We refer to $J(k, c, s)$ as Van Loan's Givens rotation. Van Loan's Householder and Givens transformations are both orthogonal and symplectic. It is worth noting that for $i \neq k$ and $i \neq n+k$, we have $J(k, c, s)e_i = e_i$. Also, we have $J(k, c, s)e_k = ce_k - se_{n+k}$ and $J(k, c, s)e_{n+k} = se_k + ce_{n+k}$. Thus, $J(k, c, s)$ applied to a vector a , leaves unchanged all the rows of $J(k, c, s)a$ except rows k and $n+k$. It is obvious also that $H(k, w)e_i = e_i$ for $i = 1, \dots, k-1$ and $i = n+1, \dots, n+k-1$. The modification of the even sub-steps of JHOSH (or JHSH) algorithm is as follows. Let $A = [a_1, \dots, a_n, a_{n+1}, \dots, a_{2n}] \in \mathbb{R}^{2n \times 2n}$ be a given matrix and set $A^{(0)} = A$. The first sub-step is obtained by creating the desired zeros in the first column, via the H_1 as above. The updated matrix is $A^{(1)}$. Now, for creating the desired zeros in the column $n+1$ and keeping the first column unchanged, we shall use the Van Loan's transformations, instead of H_2 . For $k = n, \dots, 2$, we compute $J(k, c, s)$ such that a zero is created in position $n+k$ in the $n+1$ th column of $J(k, c, s)A^{(1)}$. The first column as well as the already created zeros in the current $n+1$ column of $A^{(1)}$ remain unchanged. The first

and the $n + 1$ th columns of $J(k, c, s)A^{(1)}$ leave unchanged when the latter is multiplied on the right by $J(k, c, s)^T$. The matrix $A^{(1)}$ is then updated with $A^{(2)} = J(k, c, s)A^{(1)}J(k, c, s)^T$. So the entries at positions $n + 2, \dots, 2n$ in the $n + 1$ column of $A^{(2)}$ are zeros. Now, we compute w so that the action of Van Loan's Householder in the product $H(2, w)A^{(2)}$ creates zeros in the positions $3, \dots, n$ in the $n + 1$ column. The first column of $H(2, w)A^{(2)}$ as well as the already created zeros remain unchanged. The transformation $H(2, w)$ leaves unchanged the first and the $n + 1$ columns of the updated matrix $A^{(2)} = H(2, w)A^{(2)}H(2, w)^T$.

At the j th step, the first sub-step is obtained by creating the desired zeros in the j th column, via the H_{2j-1} as in JHOSH. The updated matrix is $A^{(2j-1)}$. Now, the desired zeros in the column $n + j$ are created by using the Van Loan's givens rotations, instead of H_{2j} . For $k = n, \dots, j + 1$, we compute $J(k, c, s)$ such that a zero is created in position $n + k$ in the $n + j$ th column of $J(k, c, s)A^{(2j-1)}$. The columns $1, \dots, j$ and $n + 1, \dots, n + j - 1$ as well as the already created zeros in the current $n + j$ column of $A^{(2j-1)}$ remain unchanged. The columns $1, \dots, j$ and $n + 1, \dots, n + j$ of $J(k, c, s)A^{(2j-1)}$ leave unchanged when the latter is multiplied on the right by $J(k, c, s)^T$. The matrix $A^{(2j-1)}$ is then updated with $A^{(2j)} = J(k, c, s)A^{(2j-1)}J(k, c, s)^T$. So the entries at positions $n + j + 1, \dots, 2n$ in the $n + j$ column of $A^{(2j)}$ are zeros. Now, we compute w so that the action of Van Loan's Householder in the product $H(j + 1, w)A^{(2j)}$ creates zeros in the positions $j + 2, \dots, n$ in the $n + j$ th column. The columns $1, \dots, j$ and $n + 1, \dots, n + j - 1$ as well as the already created zeros in the current $n + j$ column of $A^{(2j)}$ remain unchanged. $H(j + 1, w)$ leaves unchanged the columns $1, \dots, j$ and $n + 1, \dots, n + j$ of the updated matrix $A^{(2j)} = H(j + 1, w)A^{(2j)}H(j + 1, w)^T$. We obtain the following algorithm

Algorithm 10. *function* $[S, H] = \text{JHMSH}(A)$

```

    twon = size( $A(:, 1)$ );  $n = \text{twon}/2$ ;  $S = \text{eye}(\text{twon})$ ;
    for  $j = 1 : n - 1$ 
         $J = [\text{zeros}(n - j + 1), \text{eye}(n - j + 1); -\text{eye}(n - j + 1), \text{zeros}(n - j + 1)]$ ;
         $ro = [j : n, n + j : 2n]$ ;  $co = [j : n, n + j : 2n]$ ;
         $[c, v] = \text{osh2}(A(ro, j))$ ;
    % Updating  $A$  :
         $A(ro, co) = A(ro, co) + c * v * (v' * J * A(ro, co))$ ;
         $A(:, co) = A(:, co) - (A(:, co) * (c * v)) * v' * J$ ;
    % Updating  $S$  (if needed):
```

```

 $S(:, co) = S(:, co) - c * S(:, co) * (v * v') * J;$ 
for  $k = 2n : n + j + 1,$ 
 $[c, s] = vlg(k, A(:, n + j)),$ 
%Updating A:

$$\begin{bmatrix} A(k, co) \\ A(n + k, co) \end{bmatrix} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} A(k, co) \\ A(n + k, co) \end{bmatrix};$$


$$\begin{bmatrix} A(:, k) & A(:, n + k) \end{bmatrix} = \begin{bmatrix} A(:, k) & A(:, n + k) \end{bmatrix} \begin{bmatrix} c & -s \\ s & c \end{bmatrix};$$

%Updating S (if needed):

$$\begin{bmatrix} S(:, k) & S(:, n + k) \end{bmatrix} = \begin{bmatrix} S(:, k) & S(:, n + k) \end{bmatrix} \begin{bmatrix} c & -s \\ s & c \end{bmatrix};$$

end
if  $j \leq n - 2$ 
 $[\beta, w] = vlh(j + 1, A(:, n + j));$ 
%Updating A:
 $A(j + 1 : n, co) = A(j + 1 : n, co) - \beta * w * w' * A(j + 1 : n, co)$ 
 $A(j + 1 + n : 2n, co) = A(j + 1 + n : 2n, co) - \beta * w * w' * A(j + 1 + n : 2n, co);$ 
 $A(:, j + 1 : n) = A(:, j + 1 : n) - \beta * A(:, j + 1 : n) w * w';$ 
 $A(:, n + j + 1 : 2n) = A(:, n + j + 1 : 2n) - \beta * A(:, n + j + 1 : 2n) w * w';$ 
%Updating S (if needed):
 $S(:, j + 1 : n) = S(:, j + 1 : n) - \beta * S(:, j + 1 : n) w * w';$ 
 $S(:, n + j + 1 : 2n) = S(:, n + j + 1 : 2n) - \beta * S(:, n + j + 1 : 2n) w * w';$ 
end
end
end

```

Algorithm 11. $function[c, s] = vlg(k, a)$

```

%  $a = [a_1, \dots, a_{2n}]$ .
 $twon = length(a); n = twon/2;$ 
 $r = \sqrt{a_k^2 + a_{n+k}^2};$ 
if  $r = 0$  then  $c = 1; s = 0;$ 
else  $c = \frac{a_k}{r}; s = \frac{a_{n+k}}{r};$ 
end

```

Algorithm 12. $function[\beta, w] = vlh(k, a)$

```

%  $a = [a_1, \dots, a_{2n}]$ .
 $twon = length(a); n = twon/2;$ 

```

```

% w = (w1, ..., wn-k+1)T;
r1 = ∑i=2n-k+1 ai+k-12;
r = √(ak2 + r1);
w1 = ak + sign(ak)r;
wi = ai+k-1 for i = 2, ..., n - k + 1;
r = w12 + r1; β =  $\frac{2}{r}$ ;
% P = I - βwwT; (H(k, w)a)i = 0 for i = k + 1, ..., n.
end

```

4. Numerical experiments

In this work, our goal was to introduce an new algorithm for computing a J -Hessenberg reduction of a matrix, via symplectic Householder transformations, which are rank-one modification of the identity. We showed how this reduction may be handled. The reduction process involves free parameters. We outlined how some optimal choice can be done, which gave rise to JHOSH algorithm. In order to enforce accuracy, we succeed to modify the JHOSH algorithm, by replacing half of the involved symplectic transformations with other transformations, which are both orthogonal and symplectic. This gave rise to JHMSH algorithm, which behaves with satisfactory properties and is better than all the previous ones. The algorithms JHESS as well as JHSH and its different variants JHOSH, JHMSH may meet breakdowns/near-breakdowns. Such breakdowns/near-breakdowns occur exactly in the same condition for all these algorithms. This gives rise to very important questions concerning for example the different strategies for curing, when it is possible, such breakdowns/near-breakdowns. For example, a breakdown is encountered in JHMSH algorithm when for a certain call, the function *osh2* returns $\xi \neq 0$ and $\nu = 0$. A near-breakdown occurs when $\xi \neq 0$, $\nu \neq 0$ and the ration ξ/ν is very large. An extended and detailed study is needed. This will be the focus of a forthcoming paper.

We propose here a numerical example, allowing us the comparison between the different algorithms.

Example : Let us take $A = randn(2n)$ and run JHESS, JHMSH, JHOSH. The loss of J -orthogonality and the error in the J -Hessenberg reduc-

Loss of J -orthogonality $\ I - S^J S\ _2$			
$2n$	<i>JHESS</i>	<i>JHMSH</i>	<i>JHOSH</i>
4	$2.2377e - 16$	$5.0453e - 16$	$1.3878e - 16$
6	$1.2362e - 15$	$1.0314e - 14$	$7.8665e - 15$
8	$1.1262e - 15$	$4.4185e - 15$	$8.2489e - 15$
10	$5.5159e - 15$	$6.6951e - 14$	$2.3061e - 13$
12	$8.3091e - 15$	$8.3005e - 13$	$7.7104e - 13$
14	$5.5932e - 14$	$4.5568e - 13$	$8.9718e - 11$
16	$1.4082e - 14$	$2.0836e - 13$	$5.9120e - 12$
18	$2.8530e - 14$	$1.5159e - 12$	$1.8129e - 10$
20	$1.5660e - 13$	$8.1831e - 11$	$1.9407e - 09$
22	$1.6207e - 14$	$3.0169e - 13$	$8.4138e - 11$
24	$6.5797e - 14$	$9.3572e - 12$	$8.0934e - 09$
26	$1.2295e - 13$	$3.9518e - 11$	$1.0048e - 05$
28	$4.5993e - 14$	$1.6715e - 12$	$1.6731e - 09$
30	$6.1491e - 13$	$5.9323e - 11$	$2.8166e - 05$

Table 1: Loss of J -orthogonality, $A = randn(2n)$.

tion, for the different algorithms, are displayed in Table 1 and Table 2 respectively. One can observe that JHESS and JHMSH provide sensibly similar results. This is explained by the fact that both use a half of orthogonal and symplectic transformations (numerically stables) and another half of transformations which are only symplectic (but not orthogonal). We emphasize that the backward error $\|A - SHS^J\|$ and the forward error $\|H - S^J A S\|$ of JHMSH (respectively JHESS) are of the same order of magnitude. Also, JHOSH presents a significant disadvantage compared to JHESS and JHMSH. This is not surprising since JHOSH uses only symplectic but not orthogonal transformations. Such transformations may be the source of numerical instability. This is the case when these transformations have a large 2-condition number, which corresponds to the presence of a near-breakdown.

5. Conclusion

In this paper, we introduce a reduction of a matrix to the upper J -Hessenberg form, based on the symplectic Householder transformations, which are rank-one modification of the Identity. This reduction is the crucial step for constructing an efficient SR-algorithm. The method is the analogue of

Error of J -Hessenberg reduction			$\ H - S^J AS\ _2$
$2n$	$JHESS$	$JHMSH$	$JHOSH$
4	$7.6284e - 16$	$1.7280e - 15$	$1.4299e - 15$
6	$1.1399e - 14$	$1.3724e - 13$	$4.4936e - 13$
8	$5.4087e - 15$	$2.7576e - 14$	$8.9172e - 14$
10	$4.1767e - 14$	$2.6532e - 12$	$1.2819e - 11$
12	$4.9776e - 14$	$7.1119e - 12$	$2.0655e - 11$
14	$1.7671e - 13$	$1.3752e - 11$	$6.4185e - 09$
16	$1.2971e - 13$	$1.4069e - 12$	$2.1820e - 10$
18	$1.7410e - 13$	$6.4203e - 12$	$3.1054e - 08$
20	$1.6234e - 12$	$3.3818e - 09$	$7.7719e - 07$
22	$1.2996e - 13$	$7.0366e - 12$	$2.4491e - 09$
24	$7.4530e - 13$	$3.1000e - 10$	$7.4156e - 07$
26	$1.2377e - 12$	$1.2405e - 09$	$6.3300e - 02$
28	$7.0871e - 13$	$1.8094e - 11$	$4.9546e - 07$
30	$3.9641e - 12$	$1.4573e - 09$	$1.1500e - 02$

Table 2: Error of J -Hessenberg reduction, $A = randn(2n)$

the reduction of a matrix to Hessenberg form, via Householder transformations, when instead of an Euclidean linear space, one takes a symplectic one. Then the algorithm JHOSH is derived, corresponding to an optimal choice of the free parameters. Furthermore, JHOSH is significantly improved by showing that half of these symplectic Householder transformations may be replaced by Van Loan's symplectic and orthogonal transformations leading to a variant JHMSH which is significantly more stable numerically. The algorithm JHMSH behave quite similarly to JHESS algorithm. Moreover, both may meet fatal breakdown at the same condition. The treatment of breakdowns/near-breakdowns and related topics deserve more investigations and will be the focus of a forthcoming work.

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