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Symplectic Householder transformations for a *QR*-like decomposition, a geometric and algebraic approaches

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Abstract

The aim of this paper is to show how geometric and algebraic approaches lead us to a new symplectic elementary transformations: the 2-D symplectic Householder transformations. Their features are studied in details. Their interesting properties allow us to construct a new algorithm for computing a *SR* factorization. This algorithm is based only on these 2-D symplectic Householder transformations. Its new features are highlighted. The study shows that, in the symplectic case, the new algorithm is the corresponding one to the classical *QR* factorization algorithm, via the Householder transformations. Some numerical experiments are given.

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1. Introduction

Householder transformations [7,18] play an important role in numerical linear algebra. Their interesting features are widely used for constructing efficient and stable [8] algorithms. Thus, for example, the well-known *QR* factorization, via Householder transformations, is used for solving a large variety of problems as linear systems, least squares problems, eigenvalue problems, matrix factorization [2,7,14,18]. From a geometric algebra point of view, the usual Householder transformation is a transvection [1] of a finite dimensional Euclidean linear space **E**, which in addition, belongs to the group of isometries. An isometry is an isomorphism that preserves the scalar product. The group **G** of isometries is also called the orthogonal group. In matrix language, the orthogonal group is the group of orthogonal (or Hermitian) matrices. It provides similarity transformations, structure-preserving, for Jordan and Lie algebras.

Some important applications in control theory, lead to Hamiltonian or skew-Hamiltonian matrices, which are structured matrices [9,10,12,13,17]. Unfortunately, such structures are not preserved under orthogonal (or Hermitian) similarities. However, these structures are preserved by symplectic similarities. The group of symplectic transfor-

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mations can be interpreted as the group of isometries of a finite dimensional symplectic linear space **F** [1]. We refer to as the symplectic group **S**.

The corresponding Jordan algebra (respectively, Lie algebra) is nothing else than the algebra of the skew-Hamiltonian matrices (respectively, the Hamiltonian matrices). The *SR* decomposition [3,4,6,13] is the basis for constructing structure-preserving methods for Hamiltonian or skew-Hamiltonian matrices. It can be obtained using symplectic Gram–Schmidt [6,15,16] algorithm or a *QR*-like factorization using symplectic elementary transformations [5,17,13].

In this paper, the geometric approach leads us to the skew-Hamiltonian 2-D symplectic Householder transformations. Their properties are studied in details. The algebraic approach is more complete and general. The approach is based on the following result: any finite dimensional symplectic linear space possesses a canonical splitting in a direct sum of symplectic planes. The approach leads us to the 2-D symplectic Householder transformations. Their features are established in details. Such transformations will serve to construct an algorithm for computing a *SR* factorization. The new algorithm is the corresponding one, in the symplectic case, to the *QR* factorization via Householder transformations, in the Euclidean case.

The remainder of this paper is organized as follows. In Section 2, we introduce some notations, some definitions and results. Section 3 describes briefly the symplectic geometry. In Section 4, the geometric approach is presented. A detailed study is derived. The algebraic approach is treated in Section 5. Interesting new results are given. Section 6 deals with the construction of a *SR* decomposition via the 2-DSH transformations. Some numerical experiments are reported. Section 7 is devoted to concluding remarks.

2. Notations and some preliminaries

In this section, we recall some notations and necessary tools which will be used throughout this paper.

2.1. Notations

We use italic capital and lower letters to denote matrices and vectors, respectively. The transpose of a matrix $M=(m_{ij})$ is denoted by $M^{\mathrm{T}}=(m_{ji})$. The range of M (i.e., the linear space, spanned by the columns of M) is denoted by $\mathrm{ran}(M)$ and the usual scalar product by $(x, y) = x^{\mathrm{T}} y$. We set

$$J_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}, \tag{2.1}$$

where 0_n and I_n denote the null and the identity matrices of $\mathbb{R}^{n\times n}$, respectively. The matrix J_{2n} is skew-symmetric and orthogonal. If the actual dimensions of the matrices are apparent from the context, we will write simply $0, I, J$. We also use the notation

$$\mathrm{diag}(K_1, \ldots, J_p) = \begin{pmatrix} K_1 & & \\ & \ddots & \\ & & K_p \end{pmatrix},$$

where the dimension will be apparent from the context.

2.2. Scalar product associated to the matrix J

Consider the bilinear form $(x, y) \mapsto (x, y)_J$ from $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$ to $\mathbb{R}$ defined by

$$\forall x \in \mathbb{R}^{2n}, \quad \forall y \in \mathbb{R}^{2n}, \quad (x, y)_J = (x, Jy) = x^{\mathrm{T}} J y. \tag{2.2}$$

The form is non-degenerate, i.e.,

$$(x, y)_J = 0, \quad \forall y \Longrightarrow x = 0 \tag{2.3}$$

and is skew-symmetric, i.e.,

$$\forall x, y \in \mathbb{R}^{2n}, \quad (x, y)_J = -(y, x)_J. \tag{2.4}$$

For any real $2n$-by-$2n$ matrix M, there is a unique matrix M^J, the adjoint of M with respect to $(\cdot,\cdot)_J$ defined by

$$\forall x, y \in \mathbb{R}^{2n}, \quad (Mx, y)_J = (x, M^J y)_J. \tag{2.5}$$

It is easy to show that

$$M^J = J^{\mathrm{T}} M^{\mathrm{T}} J. \tag{2.6}$$

The following properties of the adjoint with respect to $(\cdot,\cdot)_J$ are all analogous to properties of transpose. We have obviously: $\forall M, N \in \mathbb{R}^{2n\times 2n}$,

$$(M+N)^J = M^J + N^J, \quad (MN)^J = N^J M^J, \quad (M^J)^J = M, \quad (M^J)^{\mathrm{T}} = (M^{\mathrm{T}})^J. \tag{2.7}$$

A linear space equipped with the underlying skew-symmetric inner product $(\cdot,\cdot)_J$ is called symplectic linear space.

Let us recall that the symplectic group is given by

$$\begin{aligned}\mathbf{S} &= \{S \in \mathbb{R}^{2n\times 2n} \mid (Sx, Sy)_J = (x, y)_J, \forall x, y \in \mathbb{R}^{2n}\}\\ &= \{S \in \mathbb{R}^{2n\times 2n} \mid S^J S = I\},\end{aligned}$$

the Jordan algebra $\mathbf{J}$ is given by

$$\begin{aligned}\mathbf{J} &= \{A \in \mathbb{R}^{2n\times 2n} \mid (Ax, y)_J = (x, Ay)_J, \forall x, y \in \mathbb{R}^{2n}\}\\ &= \{A \in \mathbb{R}^{2n\times 2n} \mid A^J = A\},\end{aligned}$$

and the Lie algebra is given by

$$\begin{aligned}\mathbf{L} &= \{H \in \mathbb{R}^{2n\times 2n} \mid (Hx, y)_J = -(x, Hy)_J, \forall x, y \in \mathbb{R}^{2n}\}\\ &= \{H \in \mathbb{R}^{2n\times 2n} \mid H^J = -H\}.\end{aligned}$$

A matrix S in $\mathbf{S}$ is called symplectic, a matrix A in $\mathbf{J}$ is called skew-Hamiltonian and a matrix H in $\mathbf{L}$ is called Hamiltonian. The symplectic group $\mathbf{S}$ provides structure-preserving similarities for matrices in $\mathbf{S}$, $\mathbf{J}$, and $\mathbf{L}$ [10], i.e.,

$$\forall S \in \mathbf{S}, \quad A \in \mathbf{E} \Longrightarrow S^{-1}AS \in \mathbf{E} \quad \text{where } \mathbf{E} = \mathbf{S}, \mathbf{J}, \text{ or } \mathbf{L}.$$

2.3. Extensions

In the literature, symplectic matrices are defined as elements of the symplectic group $\mathbf{S}$. This definition is extended [15] to matrices which are not necessarily square but only of size $2n \times 2k$. An extension of the definition of the adjoint is needed. The adjoint of $x \in \mathbb{R}^{2n}$ is defined by

$$x^J = x^{\mathrm{T}} J, \tag{2.8}$$

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

$$M^J = J_{2k}^{\mathrm{T}} M^{\mathrm{T}} J_{2n}. \tag{2.9}$$

Thus, in particular, the underlying inner product can be written as

$$(x, y)_J = x^J y. \tag{2.10}$$

Definition 2.1. A matrix $S \in \mathbb{R}^{2n\times 2k}$ is called symplectic if

$$S^J S = I_{2k}. \tag{2.11}$$

The non-square adjoint (2.9) of M with respect to $(\cdot,\cdot)_J$ satisfies $\forall M \in \mathbb{R}^{2n\times 2k}$, $\forall N \in \mathbb{R}^{2k\times 2p}$

$$(MN)^J = N^J M^J, \quad (M^J)^J = M, \quad (M^J)^{\mathrm{T}} = (M^{\mathrm{T}})^J. \tag{2.12}$$

For proof and more details see [15].

We give the following lemma, which will be used in the sequel.

Lemma 2.2. *Let $V = [v_1, v_2]$ be a $2n \times 2$ real matrix and Σ be a 2×2 real matrix, then we get*

$$\Sigma + \Sigma^J = \mathrm{trace}(\Sigma) I_2, \quad \Sigma\Sigma^J = \det(\Sigma) I_2 \quad \textit{and} \quad V^J V = v_1^{\mathrm{T}} J v_2 I_2.$$

Proof. Set

$$\Sigma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

Then

$$\Sigma^J = J^{\mathrm{T}} \Sigma^{\mathrm{T}} J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

It follows that $\Sigma + \Sigma^J = \mathrm{trace}(\Sigma) I_2$ and $\Sigma\Sigma^J = \det(\Sigma) I_2$. We get obviously

$$V^J V = J^{\mathrm{T}} V^{\mathrm{T}} J V = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} v_1^{\mathrm{T}} \\ v_2^{\mathrm{T}} \end{pmatrix} J \begin{pmatrix} v_1 & v_2 \end{pmatrix} = v_1^{\mathrm{T}} J v_2 I_2. \qquad \square$$

3. Symplectic geometry

In the sequel, we need to consider the specificity of the symplectic geometry. We outline briefly some features of symplectic geometry contrasting with orthogonal geometry. See [1,15] for more details on common features of orthogonal and symplectic geometry and on special features of symplectic geometry. As usual, a vector $x \in \mathbb{R}^{2n}$ is said to be orthogonal to $y \in \mathbb{R}^{2n}$, with respect to the skew-symmetric scalar product $(\cdot,\cdot)_J$, iff $(x, y)_J = 0$. We use the symbol $\perp$ for the orthogonality in an Euclidean space whereas $\perp'$ is used for a symplectic space. Let $\mathscr{L}$ be a linear subspace of $\mathbb{R}^{2n}$. Define the symplectic complement of $\mathscr{L}$ to be the subspace

$$\mathscr{L}^{\perp'} = \{x \in \mathbb{R}^{2n} | \forall y \in \mathscr{L}, (x, y)_J = 0\}.$$

The symplectic complement satisfies

$$(\mathscr{L}^{\perp'})^{\perp'} = \mathscr{L}^{\perp'} \tag{3.1}$$

and

$$\dim \mathscr{L} + \dim \mathscr{L}^{\perp'} = 2n. \tag{3.2}$$

However, unlike orthogonal complements, $\mathscr{L}^{\perp'} \cap \mathscr{L}$ does not need to be the null space. We recall the following case:

- $\mathscr{L}$ is symplectic if
$$\mathscr{L}^{\perp'} \cap \mathscr{L} = \{0\}. \tag{3.3}$$
This is true iff the restriction of $(\cdot,\cdot)_J$ on $\mathscr{L}$ is a non-degenerate form.
- $\mathscr{L}$ is isotropic [1] if
$$\mathscr{L}^{\perp'} \cap \mathscr{L} = \mathscr{L}. \tag{3.4}$$

This is true iff the restriction of $(\cdot,\cdot)_J$ on $\mathscr{L}$ is the null form. Indeed, any one-dimensional subspace is isotropic.

In Euclidean spaces, there exists no isotropic subspaces different from the zero space, whereas there are in symplectic spaces.

Any finite Euclidean space $\mathbf{E}$, can be written as a direct sum of a given one-dimensional subspace (line) and its orthogonal complement, i.e.,

$$\forall v \in \mathbf{E}\backslash\{0\}, \quad \mathbf{E} = \langle v \rangle \oplus \langle v \rangle^{\perp}. \tag{3.5}$$

As a consequence of (3.5), the Euclidean space $\mathbb{R}^n$ can be written as a direct sum of orthogonal lines, i.e.,

$$\exists v_1, \dots, v_n \in \mathbb{R}^n | \mathbb{R}^n = \oplus_{i=1}^n \text{span}\{v_i\}, \quad v_i \perp v_j, \ \ \forall 1 \leqslant i \neq j \leqslant n. \tag{3.6}$$

Contrasting with the Euclidean case, a symplectic linear space $\mathbb{R}^{2n}$ can never be written as a direct sum of symplectic one-dimensional subspaces (lines) as (3.6). This is due to the fact that any one-dimensional subspace is isotropic, i.e.,

$$\forall v \in \mathbf{E}, \quad \langle v \rangle \subset \langle v \rangle^{\perp'}. \tag{3.7}$$

However, such splitting is possible using two-dimensional subspaces (planes). In fact, for any $\langle v_1, v_2 \rangle$ symplectic subspace of $\mathbb{R}^{2n}$, one gets

$$\mathbb{R}^{2n} = \langle v_1, v_2 \rangle \oplus \langle v_1, v_2 \rangle^{\perp'}. \tag{3.8}$$

As a consequence of (3.8), the symplectic linear space $\mathbb{R}^{2n}$ can be written as a direct sum of symplectic planes, i.e.,

$$\exists v_i \in \mathbb{R}^{2n}, \quad i = 1, \dots, 2n \quad \text{such that,} \ \ \mathbb{R}^{2n} = \oplus_{i=1}^n \langle v_{2i-1}, v_{2i} \rangle, \tag{3.9}$$

where the matrix $[v_{2i-1}, v_{2i}]$ is symplectic, for $1 \leqslant i \leqslant n$, and

$$\forall 1 \leqslant i \neq j \leqslant n, \quad \langle v_{2i-1}, v_{2i} \rangle \perp' \langle v_{2j-1}, v_{2j} \rangle. \tag{3.10}$$

4. Geometric approach, limited case

In an Euclidean space $\mathbf{E}$, the Householder transformation

$$H_v = I - 2vv^{\mathrm{T}} / v^{\mathrm{T}} v \tag{4.1}$$

is associated to the linear splitting (3.5) and conversely. H_v is a symmetry with respect to the hyperplane $\langle v \rangle^{\perp}$, i.e.,

$$\forall x \in \langle v \rangle, \ \ Hx = -x, \quad \forall x \in \langle v \rangle^{\perp}, \ \ Hx = x. \tag{4.2}$$

In a symplectic linear space $\mathbb{R}^{2n}$, it is not permitted to follow the same scheme, for constructing a "symmetry", since

$$\langle v \rangle \subset \langle v \rangle^{\perp'}.$$

However, the linear splitting (3.8) can be associated in a natural way with the elementary transformation

$$H_V = I - 2V(V^J V)^{-1} V^J \tag{4.3}$$

and conversely, where $V = [v_1, v_2]$ and the plane $\langle v_1, v_2 \rangle$ symplectic. In a symplectic space, this transformation can be interpreted geometrically as an extended "symmetry" with respect to planes. In other words, any vector of the $\langle v_1, v_2 \rangle^{\perp'}$ remains fixed by H_V whereas any vector of $\langle v_1, v_2 \rangle$ is displaced to the opposite, i.e.,

$$\forall x \in \langle v_1, v_2 \rangle, \ \ H_V x = -x, \quad \forall x \in \langle v_1, v_2 \rangle^{\perp'}, \ \ H_V x = x. \tag{4.4}$$

Remark 4.1. Note that $\langle v_1, v_2 \rangle$ is symplectic iff $v_1^{\mathrm{T}} J v_2 \neq 0$ and H_V is defined only when $\langle v_1, v_2 \rangle$ is symplectic. Since $V^J V = v_1^{\mathrm{T}} J v_2 I_2$, then H_V can be written as

$$H_V = I - \frac{2}{v_1^{\mathrm{T}} J v_2} V V^J \quad \text{or} \quad H_V = I - 2VV^J / V^J V.$$

If $v_1^{\mathrm{T}} J v_2 = 1$ (which can be guaranteed by a adequate choice) then, the expression is reduced to $H_V = I - 2VV^J$. We will refer to V as the direction of H_V.

We establish the useful properties of H_V.

Proposition 4.2. *The elementary transformation H_V is symplectic ($H_V^J H_V = I_{2n}$) and skew-Hamiltonian ($H_V^J = H_V$).*

Proof. We get $H_V^J = (I - (2/v_1^{\mathrm{T}} J v_2) V V^J)^J = I - (2/v_1^{\mathrm{T}} J v_2)(V V^J)^J = H_V$. Then, $H_V^J H_V = H_V^2 = I - 4V(V^J V)^{-1} V^J + 4V(V^J V)^{-1} V^J V (V^J V)^{-1} V^J = I$. $\square$

Proposition 4.3. *Let G be a non-singular* 2-*by*-2 *real matrix and set $W = VG$. Then $H_V = H_W$.*

Proof. $H_W = I - 2W(W^J W)^{-1} W^J = I - 2VG(G^J V^J V G)^{-1} G^J V^J$. From Lemma 2.2, we have $G^J G = \det(G) I_2$ and $V^J V = v_1^{\mathrm{T}} J v_2 I_2$ and then we get $H_W = H_V$. $\square$

Let $\mathscr{H}_2$ be $\mathscr{H}_2 = \{H_V, V \in \mathbb{R}^{2n\times 2}, \mathrm{ran}(V) \text{ symplectic}\}$. The mapping problem for H_V consists in mapping simultaneously a pair of vectors into another pair. It takes the form

Theorem 4.4. *Let $X, Y \in \mathbb{R}^{2n\times 2}$ such that $X^J(X - Y) \neq O_2$. Then*

$$\exists H_V \in \mathscr{H}_2 \text{ such that } Y = H_V X \iff X^J X = Y^J Y, \quad Y^J X = X^J Y.$$

Moreover, the elementary symplectic transformation H_{Y-X} of direction $Y - X$ moves X into Y.

Proof. Since H_V is symplectic, we get $Y^J Y = (H_V X)^J H_V X = X^J H_V^J H_V X = X^J X$. As H_V is skew-Hamiltonian, we obtain $Y^J X = (H_V X)^J X = X^J (H_V)^J X = X^J H_V X = X^J Y$.

Reciprocally, we recall (Lemma 2.2) that $(Y - X)^J (Y - X)$ is non-singular iff $(Y - X)^J (Y - X) \neq 0_2$. From $X^J X = Y^J Y$, $Y^J X = X^J Y$, we get $(X - Y)^J Y = X^J Y - Y^J Y = Y^J X - X^J X = -(X - Y)^J X$ and then $(Y - X)^J (Y - X) = 2(X - Y)^J X \neq 0_2$. It follows that $(Y - X)^J (Y - X)$ is non-singular. We have then $H_{Y-X} X = X - 2 (Y - X)((Y - X)^J (Y - X))^{-1} (Y - X)^J X = X - 2(Y - X)(2(X - Y)^J X)^{-1} (Y - X)^J X = X + Y - X = Y$. $\square$

We refer to H_V as skew-Hamiltonian 2-D symplectic Householder transformation. In [13], Paige et al. introduced the matrix transformation

$$H(k, w) = \begin{pmatrix} \mathrm{diag}(I_{k-1}, P) & 0 \\ 0 & \mathrm{diag}(I_{k-1}, P) \end{pmatrix}, \tag{4.5}$$

where

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

The matrix $H(k, w)$ is orthogonal and symplectic. They used the denomination Householder symplectic matrix to designate $H(k, w)$, which is just a direct sum of two "ordinary" n-by-n Householder matrices [18]. It is used to zero selected components of a vector [13,17] in a skew-Hamiltonian context. We establish the following link.

Proposition 4.5. *The symplectic Householder transformation introduced by Paige et al. in* [13] *is a particular case of the skew-Hamiltonian* 2-*D symplectic Householder transformations. Furthermore, $H(k, w)$ is recovered explicitly by*

$$H(k, w) = I_{2n} - 2VV^J/V^J V,$$

with

$$V = [v_1, v_2], \quad v_2 = J^{\mathrm{T}} v_1, \quad v_1 = (0 \quad w| \quad 0 \quad 0)^{\mathrm{T}}.$$

Proof. From $v_1 = (0 \quad w| \quad 0 \quad 0)^{\mathrm{T}}$ and $v_2 = J^{\mathrm{T}} v_1 = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} v_1 = (0 \quad 0| \quad 0 \quad w)$, we get $V^J V = v_1^{\mathrm{T}} J v_2 I_2 = \|v_1\|_2^2 \, I_2 = \|w\|_2^2 \, I_2$. We have also

$$VV^J = V \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} V^{\mathrm{T}} \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & ww^{\mathrm{T}} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & ww^{\mathrm{T}} \end{pmatrix}.$$

It follows then that $I_{2n} - 2VV^J/V^J V = H(k, w)$. $\square$

The above geometric approach allowed us to construct the skew-Hamiltonian 2-D symplectic Householder transformations. They can be used in a more general context than those introduced by Paige et al. However, their context remains still limited. The following approach permits us to construct elementary symplectic transformations for a general context.

5. Algebraic approach, general case

In the sequel, we present a complete algebraic approach, leading us to an elementary symplectic transformations: the 2-D symplectic Householder transformations. These transformations will serve to present an algorithm for computing a *SR* factorization of at least almost any arbitrary matrix A. The obtained algorithm corresponds to the *QR* factorization via Householder transformations in the Euclidean case.The approach is as follows.

5.1. 2-D transvections

Set $E_i = [e_i \ e_{n+i}]$ for $i = 1, \ldots, n$ and $\kappa_2 = \mathbb{R}^{2\times 2}$. The canonical basis of $\mathbb{R}^{2n}$ is denoted by $\{e_i\}_{i=1,\ldots,2n}$. It is easy to verify that

$$E_i^{\mathrm{T}} E_j = E_i^J E_j = \delta_{ij} I_2. \tag{5.1}$$

The space $\mathbb{R}^{2n\times 2}$ can be considered as a right linear space over κ_2, of dimension n, i.e., any $U \in \mathbb{R}^{2n\times 2}$ can be expressed, in a unique way, as a right linear combination

$$U = \sum_{i=1}^{n} E_i M_i \quad \text{where } M_i = E_i^{\mathrm{T}} U = E_i^J U \in \kappa_2. \tag{5.2}$$

Definition 5.1. $\phi : \mathbb{R}^{2n\times 2} \longrightarrow \kappa_2$ is said to be a right linear form (r.l.f) if

$$\forall X, Y \in \mathbb{R}^{2n\times 2}, \ \forall \lambda \in \kappa_2, \quad \phi(X + Y\lambda) = \phi(X) + \phi(Y)\lambda. \tag{5.3}$$

Definition 5.2. T is said to be a 2-D transvection of direction V if T is of the form

$$T(X) = X + V\phi(X). \tag{5.4}$$

Lemma 5.3. *ϕ is a r.l.f* $\Longleftrightarrow \exists W \in \mathbb{R}^{2n\times 2}$ *such that* $\phi(X) = W^J X, \forall X \in \mathbb{R}^{2n\times 2}$.

Proof. Let X be $X = \sum_{i=1}^{n} E_i M_i$ with $M_i \in \mathbb{R}^{2\times 2}$. Setting $\phi(E_i) = N_i^J$, then $\phi(X) = \sum_{i=1}^{n} N_i^J M_i = (\sum_{i=1}^{n} E_i N_i)^J (\sum_{i=1}^{n} E_i M_i) = W^J X$, with $W = \sum_{i=1}^{n} E_i N_i$. □

5.2. 2-D symplectic Householder transformations (2-DSH)

Definition 5.4. H is said to be a 2-D symplectic Householder transformation of direction V if H is a symplectic 2-D transvection.

Let $\mathscr{T}_2(\mathbb{R}^{2n})$ the set of such transformations. The following theorem specifies the form of a 2-DSH.

Theorem 5.5. *H is a 2-D symplectic Householder of direction $V \neq 0$ iff there exists $\Sigma \in \kappa_2$ such that*

$$H = I + V\Sigma^J V^J, \tag{5.5}$$

with

$$\operatorname{rank}(V) = 1 \ \textit{or} \ V^J V \ \det(\Sigma) + \operatorname{trace}(\Sigma) = 0. \tag{5.6}$$

Proof. From Definition 5.4 and Lemma 5.3, the form of a 2-D symplectic Householder transformation H is given by $H = I + VW^J$ where $V, W \in \mathbb{R}^{2n\times 2}$. H is symplectic iff $H^J H = I$ which is equivalent to

$$VW^J + WV^J + WV^J VW^J = 0. \tag{5.7}$$

If $\operatorname{rank}(W) = 2$, then $\operatorname{rank}(W^J(W^J)^{\mathrm{T}}) = 2$ and $W^J(W^J)^{\mathrm{T}} \in \kappa_2$ is non-singular. Using (5.7), we get

$$V = W\Sigma^J, \tag{5.8}$$

where $\Sigma^J \in \kappa_2$ and is given by

$$\Sigma^J = -(V^J + V^J VW^J)(W^J)^{\mathrm{T}}(W^J(W^J)^{\mathrm{T}})^{-1}. \tag{5.9}$$

It follows then that $H = I + W\Sigma^J W$ which is the desired form.

If $\operatorname{rank}(W) = 1$, we get $WV^J VW^J = 0$. In the fact, setting $V = [v_1, v_2]$ and $W = [\alpha w_1, \beta w_1]$, where $w_1 \neq 0$ and ($\alpha \neq 0$ or $\beta \neq 0$). We obtain

$$WW^J = [\alpha w_1, \beta w_1]\begin{bmatrix} -\beta w_1^{\mathrm{T}} \\ \alpha w_1^{\mathrm{T}} \end{bmatrix}, \quad J = 0.$$

From Lemma 2.2, we get

$$WV^J VW^J = v_1^{\mathrm{T}} J v_2 WW^J = 0.$$

Moreover, Eq. (5.7) becomes

$$VW^J + WV^J = 0. \tag{5.10}$$

Developing (5.10), we have

$$[v_1, v_2]\begin{pmatrix} 0 & -1 \\ 1, & 0 \end{pmatrix}\begin{bmatrix} \alpha w_1^{\mathrm{T}} \\ \beta w_1^{\mathrm{T}} \end{bmatrix} + [\alpha w_1, \beta w_1]\begin{pmatrix} 0 & -1 \\ 1, & 0 \end{pmatrix}\begin{bmatrix} \alpha v_1^{\mathrm{T}} \\ \beta v_2^{\mathrm{T}} \end{bmatrix} = 0,$$

which is equivalent to

$$(-\beta v_1 + \alpha v_2)w_1^{\mathrm{T}} = w_1(-\beta v_1 + \alpha v_2)^{\mathrm{T}}. \tag{5.11}$$

If $-\beta v_1 + \alpha v_2 \neq 0$, then from (5.11), we get $w_1 = \delta(-\beta v_1 + \alpha v_2)$ for a certain $\delta \in \mathbb{R}$ and then $W = V\Sigma^J$ for a certain $\Sigma \in \kappa_2$ and one gets the desired form.

If $-\beta v_1 + \alpha v_2 = 0$, we will show that $VW^J = 0$ and then H is reduced to the identity. Therefore, we get the desired form, with $\Sigma^J = 0 \in \kappa_2$. In fact, there is no loss of generality, if one takes $\alpha = 1$. It follows

$$VW^J = [v_1, \beta v_1]\begin{pmatrix} 0 & -1 \\ 1, & 0 \end{pmatrix}\begin{bmatrix} w_1^{\mathrm{T}} \\ \beta w_1^{\mathrm{T}} \end{bmatrix} J = 0.$$

Thus the expression of any 2-DSH of direction V is necessarily given under the form

$$H = I + V\Sigma^J V. \tag{5.12}$$

Now, from (5.12), H is symplectic ($H^J H = I$) is expressed by

$$V(\Sigma^J + \Sigma + \Sigma V^J V\Sigma^J)V^J = 0. \tag{5.13}$$

From Lemma 2.2, Eq. (5.13) can be written as

$$V[\operatorname{trace}(\Sigma) + v_1^{\mathrm{T}} J v_2 \det(\Sigma)]I_2 V^J = 0. \tag{5.14}$$

It follows then that H is symplectic iff

$$VV^J = 0 \text{ or } \operatorname{trace}(\Sigma) + v_1^{\mathrm{T}} J v_2 \det(\Sigma) = 0. \tag{5.15}$$

To end the proof, since $VV^J = -v_1 v_2^{\mathrm{T}} + v_2 v_1^{\mathrm{T}}$, we get $VV^J = 0$ iff $\operatorname{rank}(V) \leqslant 1$. $\square$

Unlike for the extended "symmetry" (4.3), it is important to note that for a 2-DSH of direction V, the subspace $\mathrm{ran}(V)$ could be isotropic (i.e., $V^J V = 0$).

Remark 5.6. The 2-D symplectic Householder transformation $H = I + V\Sigma^J V^J \in \mathscr{T}_2(\mathbb{R}^{2n})$ is symplectic, but not necessarily skew-Hamiltonian.

Proposition 5.7. *$H = I + V\Sigma^J V^J \in \mathscr{T}_2(\mathbb{R}^{2n})$ let unchanged $x \in [\mathrm{ran}(V)]^{\perp'}$ and let invariant the subspace $\mathrm{ran}(V)$.*

Proof. If $x \in [\mathrm{ran}(V)]^{\perp'}$ then $V^J x = 0$ and $Hx = x$. If $x \in \mathrm{ran}(V)$ then x can be written as $x = Vz$ for a certain $z \in \mathbb{R}^2$. It follows $Hx = Vz + V\Sigma^J z = V(I_2 + \Sigma^J)z \in \mathrm{ran}(V)$. $\square$

The mapping problem for the 2-D symplectic Householder transformations is solved as follows:

Theorem 5.8. *Let $X = [x_1, x_2],\ Y = [y_1, y_2] \in \mathbb{R}^{2n\times 2}$ with $X^J X = Y^J Y \neq 0_2$. If*

$$\det((Y - X)^J X) \neq 0, \tag{5.16}$$

then

$$\exists H \in \mathscr{T}_2(\mathbb{R}^{2n}) | HX = Y.$$

Proof. Setting $H = I + (Y - X)\Sigma^J (Y - X)^J$. Then $HX = Y \iff Y - X = (Y - X)\Sigma^J (Y - X)^J X \iff (Y - X)(I_2 - \Sigma^J (Y - X)^J X) = 0$. Then (5.16) implies $\mathrm{rank}(Y - X) = 2$ and thus $(I_2 - \Sigma^J (Y - X)^J X) = 0$. Finally, we obtain $\Sigma^J = [(Y - X)^J X]^{-1}$. It is easy to verify that Σ^J satisfies the condition (5.6). $\square$

Remark 5.9. Eq. (5.16) can easily be checked since

$$\det((Y - X)^J X)) = \det((Y - X)^{\mathrm{T}} JX) = y_1^{\mathrm{T}} Jx_1 . y_2^{\mathrm{T}} Jx_2 - x_2^{\mathrm{T}} J(y_1 - x_1) . x_1^{\mathrm{T}} J(y_2 - x_2). \tag{5.17}$$

Furthermore, without the additional condition (5.16), the mapping problem takes the form

Theorem 5.10. *Let $X = [x_1, x_2],\ Y = [y_1, y_2] \in \mathbb{R}^{2n\times 2} | X^J X = Y^J Y \neq 0_2$. Then $\exists H_1 \in \mathscr{T}_2(\mathbb{R}^{2n}),\ H_2 \in \mathscr{T}_2(\mathbb{R}^{2n})$ $| H_2 H_1 X = Y$.*

Proof. If $\det((Y - X)^J X)) \neq 0$, then the result is straightforward from Theorem 5.8. Assume now that $\det((Y - X)^J X)) = 0$. There are two cases.

First case: $x_1^{\mathrm{T}} Jy_2 \neq 0$ or $x_2^{\mathrm{T}} Jy_1 \neq 0$. We choose $\alpha \in \mathbb{R}\backslash\{0, 1\}$ such that

$$x_2^{\mathrm{T}} Jy_1 + \frac{1}{\alpha} x_1^{\mathrm{T}} Jy_2 \neq 0. \tag{5.18}$$

We set $Z = [\alpha y_1, y_2/\alpha]$. It is easy to check that $Z^J Z = Y^J Y$. Then, we have

$$\det((Z - X)^J X) = x_1^{\mathrm{T}} Jy_1 . x_2^{\mathrm{T}} Jy_2 - x_1^{\mathrm{T}} J\left(\frac{y_2}{\alpha} - x_2\right) . x_2^{\mathrm{T}} J(\alpha y_1 - x_1). \tag{5.19}$$

Developing the right-hand side of Eq. (5.19) and using $\det((Y - X)^J X)) = 0$, we obtain

$$\det((Z - X)^J X) = (\alpha - 1) x_1^{\mathrm{T}} Jx_2 \left(x_2^{\mathrm{T}} Jy_1 + \frac{1}{\alpha} x_1^{\mathrm{T}} Jy_2\right) \neq 0.$$

Thus, from Theorem 5.8, there exists $H_1 \in \mathscr{T}_2(\mathbb{R}^{2n}) | H_1 X = Z$. Indeed, Z is carefully chosen since from

$$\det((Y - Z)^J Z) = z_1^{\mathrm{T}} Jy_1 . z_2^{\mathrm{T}} Jy_2 - z_1^{\mathrm{T}} J(y_2 - z_2) . z_2^{\mathrm{T}} J(y_1 - z_1),$$

and using $z_1 = \alpha y_1$, and $z_2 = y_2/\alpha$, we obtain

$$\det((Z - X)^J X) = \frac{[(\alpha - 1)(y_1^{\mathrm{T}} Jy_2)]^2}{\alpha} \neq 0.$$

Thus, from Theorem 5.8, there exists $H_2 \in \mathscr{T}_2(\mathbb{R}^{2n}) | H_2 Z = Y$, i.e., $H_2 H_1 X = Y$.

Second case: $x_1^{\mathrm{T}} J y_2 = 0$ and $x_2^{\mathrm{T}} J y_1 = 0$. We set $Z = [z_1, z_2]$, with $z_1 = x_1 + y_1$ and $z_2 = x_2$. In one hand, we have $z_1^{\mathrm{T}} J z_2 = (x_1^{\mathrm{T}} + y_1^{\mathrm{T}}) J x_2 = x_1^{\mathrm{T}} J x_2$ and thus $X^J X = Z^J Z$. On the other hand, we get

$$x_1^{\mathrm{T}} J z_2 = x_1^{\mathrm{T}} J x_2 \neq 0, \tag{5.20}$$

and

$$z_1^{\mathrm{T}} J y_2 = (x_1 + y_1)^{\mathrm{T}} J y_2 = y_1^{\mathrm{T}} J y_2 \neq 0. \tag{5.21}$$

Thus, from the first case, we have: there exists $H_1 \in \mathscr{T}_2(\mathbb{R}^{2n}) | H_1 X = Z$ (which corresponds to Eq. (5.20)) and there exists $H_2 \in \mathscr{T}_2(\mathbb{R}^{2n}) | H_2 Z = Y$ (which corresponds to Eq. (5.21)). Thus $H_2 H_1 X = Y$. $\square$

Proposition 5.11. *We have* $\mathscr{H}_2 \subset \mathscr{T}_2(\mathbb{R}^{2n})$.

Proof. Let $H \in \mathscr{H}_2$. Then, there exists $V \in \mathbb{R}^{2n\times 2}$ with $V^J V = I_2$ such that $H = I - 2VV^J$. Thus, it can be written as

$$H = I + V\Sigma^J V^J \quad \text{with } \Sigma = -2I_2.$$

Since $\Sigma = -2I_2$ satisfies (5.6), it follows that $H \in \mathscr{T}_2(\mathbb{R}^{2n})$. $\square$

In [13], Paige et al. introduced also the matrix transformation

$$J(k,\theta) = \begin{pmatrix} C & S \\ -S & C \end{pmatrix}, \tag{5.22}$$

where

$$C = \operatorname{diag}(I_{k-1}, \cos\theta, I_{n-k}), \quad S = \operatorname{diag}(0_{k-1}, \sin\theta, 0_{n-k}).$$

$J(k,\theta)$ is a Givens symplectic matrix, which is an “ordinary” $2n$-by-$2n$ Givens rotations that rotates in planes k and $k+n$ [18]. Such transformations are used [17,13] to zero prescribed entries in a vector, in a structure-preserving *QR*-like algorithm, for Hamiltonian or skew-Hamiltonian matrices. We present here the interesting result.

Proposition 5.12. *The transformation* $J(k,\theta)$ *given by* (5.22) *is a* 2-DSH.

Proof. Note first that $J(k,\theta)$ is characterized by

$$J(k,\theta)E_i = E_i \quad \text{for } i \neq k$$

and

$$J(k,\theta)E_k = E_k \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$

Consider

$$H(k,\theta) = I + E_k \Sigma^J E_k^J, \tag{5.23}$$

with

$$I_2 + \Sigma^J = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \tag{5.24}$$

In one hand, it is obvious that Σ given by (5.24) satisfies (5.6) and thus

$$H(k,\theta) \in \mathscr{T}_2(\mathbb{R}^{2n}).$$

On the other hand, since $E_k^J E_i = \delta_{ki} I_2$, we obtain

$$H(k,\theta)E_i = E_i = J(k,\theta)E_i, \quad \text{for } i \neq k$$

and

$$H(k,\theta)E_k = E_k + E_k\Sigma^J = E_k(I_2+\Sigma^J) = J(k,\theta)E_k.$$

Thus $H(k,\theta)=J(k,\theta)$. $\square$

6. *SR*-algorithm via the 2-D symplectic Householder transformations

In addition to the two types of elementary symplectic matrices $H(k,w)$ and $J(k,\theta)$ given by (4.5)–(5.22), Bunse-Gerstner et al. [5] introduced a third type defined by

$$G(k,v) = \begin{pmatrix} D & F \\ 0 & D^{-1}\end{pmatrix}, \tag{6.1}$$

where $k\in\{2,\ldots,n\}$, $v\in\mathbb{R}$ and D, F are the $n\times n$ matrices

$$D = I_n + \left(\frac{1}{(1+v^2)^{1/4}} - 1\right)(e_{k-1}e_{k-1}^{\mathrm{T}} + e_k e_k^{\mathrm{T}}),$$
$$F = \frac{v}{(1+v^2)^{1/4}}(e_{k-1}e_k^{\mathrm{T}} + e_k e_{k-1}^{\mathrm{T}}).$$

The matrix $G(k,v)$ is a non-orthogonal symplectic matrix. Such a type was introduced in order to proceed to a *SR* factorization for at least almost arbitrary matrices, i.e., up to a set of measure zero. Their algorithm is quite complicated. It involves heterogeneous transformations. It is an empirical algorithm and thus, it lacks theoretical results. There is for example no algebraic analysis behind it. The algorithm is not the corresponding one, to the classical *QR* factorization, via Householder transformations. We demonstrated here that there is no need to distinguish between $H(k,w)$ and $J(k,\theta)$ since they are just two 2-DSH.

We outline here how to obtain, in an unified way, a *SR* factorization for almost arbitrary matrices, via only 2-DSH. The introduction of $G(k,v)$ is superfluous. A 2-DSH is constructed so that one gets a *SR* factorization by following the same scheme as in *QR* factorization via Householder transformations. Thus, the new algorithm is in the symplectic case, the equivalent of *QR* factorization via Householder transformations. The new algorithm is constructed following an algebraic analysis. Theoretical results can be then established.

6.1. SR algorithm, via the 2-D symplectic Householder transformations

Let us first present the following result, which will be used in the algorithm.

Lemma 6.1. *Let U, V, W be subspaces of $\mathbb{R}^{2n}$ such that*

$$V = U\oplus W \quad with\ U\perp' W. \tag{6.2}$$

Let $\sigma_1 : U\longrightarrow U$ (respectively, $\sigma_2 : W\longrightarrow W$) a symplectic isometry.

The map $\sigma_1\perp'\sigma_2 : V\longrightarrow V$ defined by

$$\forall u\in U,\ \forall w\in W,\quad \sigma_1\perp'\sigma_2(u+w) = \sigma_1(u)+\sigma_2(w) \tag{6.3}$$

is a symplectic isometry. Moreover, if $\tau\in\mathscr{T}_2(W)$ then $I_U\perp'\tau\in\mathscr{T}_2(V)$, where I_U is the identity on U.

Proof. Let $u_1,u_2\in U$ and $w_1,w_2\in W$ and set $v_1=u_1+w_1$ and $v_2=u_2+w_2$. Set $\sigma_3=\sigma_1\perp'\sigma_2$. We have

$$\sigma_3(v_1)^J\sigma_3(v_2) = \sigma_3(v_1)^{\mathrm{T}}J\sigma_3(v_2) = (\sigma_1(u_1)+\sigma_2(w_1))^{\mathrm{T}}J(\sigma_1(u_2)+\sigma_2(w_2)).$$

From (6.2), we obtain

$$\sigma_1(u_1)^{\mathrm{T}}J\sigma_2(w_2) = \sigma_2(w_1)^{\mathrm{T}}J\sigma_1(u_2) = 0.$$

Thus

$$\sigma_3(v_1)^J\sigma_3(v_2)=\sigma_1(u_1)^{\mathrm{T}}J\sigma_1(u_2)+\sigma_2(w_1)^{\mathrm{T}}J\sigma_2(w_2).$$

Since $\sigma_1,\ \sigma_2$ are isometries, we have

$$\sigma_1(u_1)^{\mathrm{T}}J\sigma_1(u_2)=u_1^{\mathrm{T}}Ju_2 \text{ and } \sigma_2(w_1)^{\mathrm{T}}J\sigma_2(w_2)=w_1^{\mathrm{T}}Jw_2.$$

Then we obtain

$$\sigma_3(v_1)^J\sigma_3(v_2)=u_1^{\mathrm{T}}Ju_2+w_1^{\mathrm{T}}Jw_2=(u_1+w_1)^{\mathrm{T}}J(u_2+w_2)=v_1^Jv_2,$$

i.e., σ_3 is a symplectic isometry.

For $v\in V$, let $u_v\in U$, $w_v\in W$ such that $v=u_v+w_v$. Suppose that $\tau\in\mathscr{T}_2(W)$. Then τ can be written as

$$\tau=I_W+Z\Sigma^JZ^J\in\mathscr{T}_2(W),$$

for a certain $Z\in W^2$ and $\Sigma\in\kappa_2$ satisfying (5.6). Thus

$$I_U\perp'\tau(v)=u_v+\tau(w_v)=u_v+w_v+Z\Sigma^JZ^Jw_v=v+Z\Sigma^JZ^Jw_v.$$

Since $U\perp'W$, we have $Z^Ju_v=0$ and then $Z^Jw_v=Z^J(u_v+w_v)=Z^Jv$.

Therefore

$$I_U\perp'\tau(v)=(I_V+Z\Sigma^JZ^J)v.$$

It is now obvious that $I_V+Z\Sigma^JZ^J\in\mathscr{T}_2(V)$. $\square$

Let $\kappa_2^+\subset\kappa_2$ the subset of upper triangular matrices. The main steps of the algorithm can be also understood as follows. Let A be a $2n\times 2n$ matrix. AE_1 represents the first and the $n+1$th columns of A. Let Λ_1 be an arbitrary element of κ_2^+ such that $\Lambda_1^J\Lambda_1=(AE_1)^JAE_1$. The first step is

- Find $H_1\in\mathscr{T}_2(\mathbb{R}^{2n})$ such that $H_1AE_1=E_1\Lambda_1$. One uses Theorems 5.8 or 5.10 for determining explicitly $H_1=I+V_1\Sigma_1^JV_1^J$, where $V_1\in\mathbb{R}^{2n\times 2}$ and $\Sigma_1\in\kappa_2$.
  The action of H_1 on AE_1 is

$$H_1AE_1==\begin{pmatrix}\times & \times\\ 0 & 0\\ \hline 0 & \times\\ 0 & 0\end{pmatrix}=E_1\Lambda_1.$$

  Zero in the second and last rows of H_1AE_1 represents the null vector in $\mathbb{R}^{n-1}$.
- Update A by

$$H_1A=\begin{pmatrix}\times & \times & \times & \times\\ 0 & A_{11}^{(1)} & 0 & A_{12}^{(1)}\\ 0 & \times & \times & \times\\ 0 & A_{21}^{(1)} & 0 & A_{22}^{(1)}\end{pmatrix}, \tag{6.4}$$

  where $A_{ij}^{(1)}$ for $i,j=1,2$ are $n-1\times n-1$ matrices.

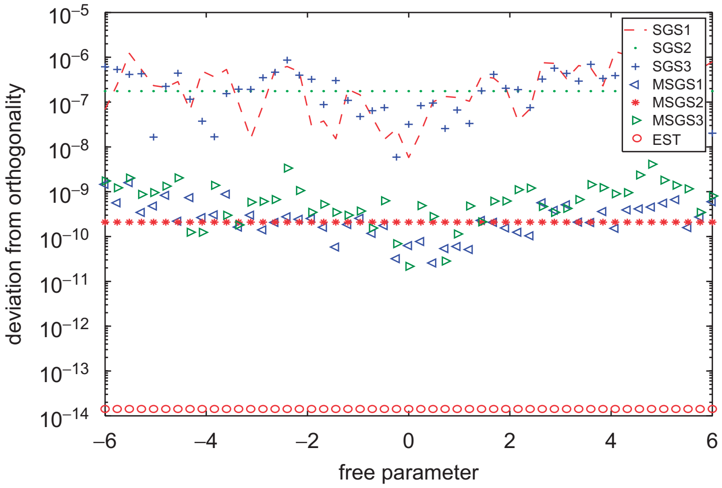

Fig. 1. pascal(8).

- Set $\tilde{A}^{(2)} = \begin{pmatrix} A_{11}^{(1)} & A_{12}^{(1)} \\ A_{21}^{(1)} & A_{22}^{(1)} \end{pmatrix}$. The second step is
- Find $\tilde{H}_2 \in \mathscr{T}_2(\mathbb{R}^{2n-2})$ so that $\tilde{H}_2\tilde{A}^{(2)}$ has the form (6.4), i.e.,

$$\tilde{H}_2\tilde{A}^{(2)} = \begin{pmatrix} \times & \times & \times & \times \\ 0 & A_{11}^{(2)} & 0 & A_{12}^{(2)} \\ 0 & \times & \times & \times \\ 0 & A_{21}^{(2)} & 0 & A_{22}^{(2)} \end{pmatrix},$$

where $A_{ij}^{(2)}$ for $i, j = 1, 2$ are $n-2 \times n-2$ matrices. Theorems 5.8 or 5.10 allow us to determine explicitly $\tilde{H}_2 = I + \tilde{V}_2\Sigma_2^J\tilde{V}_2^J$, where $\tilde{V}_2 \in \mathbb{R}^{2n-2\times 2}$ and $\Sigma_2 \in \kappa_2$. Set

$$W = \mathrm{ran}(E_1)^{\perp'}, \quad \tilde{V}_2 = \begin{pmatrix} \tilde{u}_2 \\ \hline \tilde{w}_2 \end{pmatrix}, \ V_2 = \begin{pmatrix} 0 \\ \tilde{u}_2 \\ \hline 0 \\ \tilde{w}_2 \end{pmatrix} \quad \text{and} \quad \tilde{\tilde{H}}_2 = I_W + \tilde{V}_2\Sigma_2^J\tilde{V}_2^J,$$

where $\tilde{u}_2 \in \mathbb{R}^{n-1\times 2}$, $\tilde{w}_2 \in \mathbb{R}^{n-1\times 2}$.
- We get $H_2 = I_{\mathrm{ran}(E_1)^{\perp'}}\tilde{\tilde{H}}_2 = I_{\mathbb{R}^{2n}} + V_2\Sigma_2^J V_2^J$ and then

$$H_2H_1A = \left(\begin{array}{ccc|ccc} \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & 0 & \times & \times \\ 0 & 0 & A_{11}^{(2)} & 0 & 0 & A_{12}^{(2)} \\ \hline 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & 0 & \times & \times \\ 0 & 0 & A_{21}^{(2)} & 0 & 0 & A_{22}^{(2)} \end{array}\right).$$

It is important to note that $H_2H_1AE_1 = H_1AE_1$, i.e., the first and the $n+1$th columns (respectively, rows) of H_1A are unchanged by the action of H_2. The next step is obtained in a similar way.

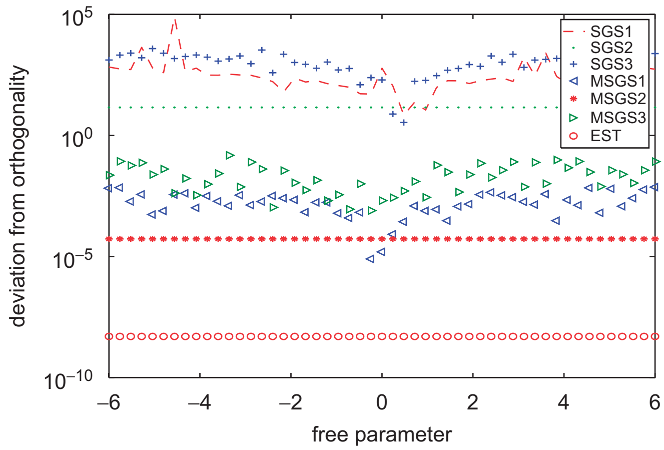

Fig. 2. pascal(14).

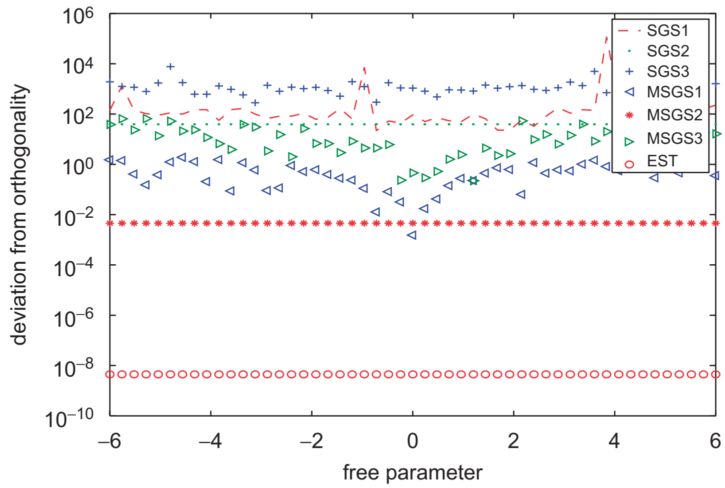

Fig. 3. pascal(16).

- At the $n-1$th step, we get

$$H_{n-1} \ldots H_2 H_1 A = R = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix},$$

where R_{11}, R_{12}, R_{21}, R_{22} are $n \times n$ upper triangular matrices. The symplectic factor S is given by $S = H_1^J H_2^J \ldots H_{n-1}^J$.

The algorithm can be easily adapted to a non-square $2n \times 2k$ matrix.

6.2. Numerical experiments

Numerical results, concerning the preservation of geometric properties of the exponential operator, when the matrix is Hamiltonian, are reported in [11]. The accuracy in the evaluation of the system energy is much higher in the proposed structure preserving method [11] than the standard Krylov process. The proposed structure preserving method uses the modified symplectic Gram–Schmidt algorithm [15] as a key step. The modified version of symplectic Gram–Schmidt algorithm presents a significant improvement with respect to the no modified version [15]. In the following numerical

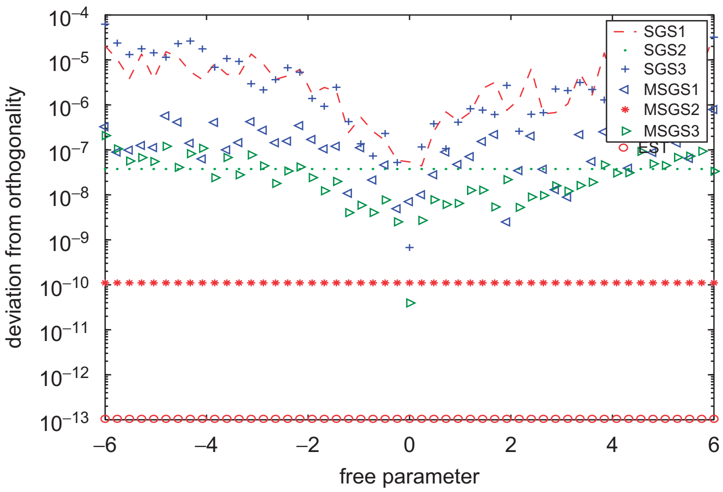

Fig. 4. rand(10).

experiments, we remark that the J-orthogonality is more preserved in a SR decomposition via 2-DSH than via the best modified version of symplectic Gram–Schmidt. Thus, we expect for example, that the preservation of the above geometric properties of the exponential operator, could be still significantly improved if an adapted SR factorization via 2-DSH is used. We mention also that we used a very simple version of the algorithm, in the sense that no particular attention was given to its optimal implementation of the algorithm. This will be the aim of future investigations (Figs. 1–4).

7. Conclusion

In this paper, a geometric approach is presented leading us to skew-Hamiltonian 2-D Householder transformations. The properties of such transformations are studied in details. However, the algebraic approach allowed us to present more general elementary symplectic Householder transformations: the 2-D symplectic Householder transformations (2-DSH). Their features are established in details, providing interesting results. A SR-algorithm based on only these 2-DSH transformations is constructed. We demonstrated that the algorithm is the corresponding one, in the symplectic case, to the QR-factorization, via Householder transformations, in the Euclidean case. The new algorithm is numerically better than the best of the modified symplectic Gram–Schmidt algorithms. Furthermore, the new algorithm is theoretically and numerically rich. These aspects will be the aim of a future work. Thus, questions as error analysis, choice of the free parameters, link with modified versions of symplectic Gram–Schmidt, breakdowns, etc., will be treated. We expect that the approach presented here will be very helpful for such investigations.

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