

ORTHOSYMMETRIC BLOCK ROTATIONS*

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Abstract. Rotations are essential transformations in many parts of numerical linear algebra. In this paper, it is shown that there exists a family of matrices unitary with respect to an orthosymmetric scalar product J , that can be decomposed into the product of two J -unitary matrices—a block diagonal matrix and an orthosymmetric block rotation. This decomposition can be used for computing various one-sided and two-sided matrix transformations by divide-and-conquer or tree-like algorithms. As an illustration, a blocked version of the QR-like factorization of a given matrix is considered.

Key words. Orthosymmetric unitary matrices, Orthosymmetric block rotations, Generalized polar decomposition, QR-like factorization, Test matrix generation.

AMS subject classifications. 15A23, 65F30.

1. Introduction. Orthosymmetric scalar products, introduced in [9] by Mackey, Mackey and Tisseur, still do not belong to the standard vocabulary of numerical linear algebra, even though they provide a unified setting for many modern structure preserving matrix tools (see for example [2, 8, 9, 10]).

Let $\mathbb{F}$ denote the field of real or complex numbers, and let $J \in \mathbb{C}^{n \times n}$ be a given nonsingular matrix that satisfies

$$(1.1) \quad J^* = \tau J, \quad |\tau| = 1,$$

for some $\tau \in \mathbb{C}$. If $J \in \mathbb{R}^{n \times n}$, then $\tau = \pm 1$. An orthosymmetric scalar product generated by J is defined by

$$(1.2) \quad [x, y] := \langle Jx, y \rangle = y^* Jx, \quad \forall x, y \in \mathbb{F}^n.$$

Obviously, this is not a scalar product in the usual sense, since J need not be Hermitian, let alone positive definite. For example, any $J = \text{diag}(\pm 1)$ satisfies (1.1), but if $J \neq \pm I$, there exist nonzero vectors x , usually called the isotropic vectors, such that $x^* Jx = 0$.

For both theory and practice, the most notable members of the class of orthosymmetric scalar products are:

*Received by the editors on September 2, 2011. Accepted for publication on March 30, 2012.
 Handling Editor: Christian Mehl.

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- (a) the Euclidean scalar product, generated by $J = \pm I$ (apart from the sign, the underlying structures are identical);
- (b) the hyperbolic scalar products, generated by $J = \text{diag}(\pm 1)$, with $J \neq \pm I$. These matrices are permutationally similar to the standard partitioned form

$$J = \text{diag}(I_m, -I_{n-m}),$$

where $0 < m < n$;

- (c) the symplectic scalar product, generated by

$$(1.3) \quad \widehat{J} = \begin{bmatrix} 0 & I_p \\ -I_p & 0 \end{bmatrix}.$$

The symplectic scalar product can also be defined by a block-diagonal matrix

$$(1.4) \quad J = \text{diag}(J_0, J_0, \dots, J_0), \quad J_0 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

The matrices $\widehat{J}$ from (1.3) and J from (1.4) of the same order $n = 2p$ are permutationally similar, i.e.,

$$(1.5) \quad P^T \widehat{J} P = J, \quad P = [e_1, e_{p+1}, e_2, e_{p+2}, \dots, e_p, e_{2p}],$$

where $e_1, \dots, e_{2p}$ is the canonical basis in $\mathbb{F}^n$.

Orthosymmetric scalar products are the broadest class of scalar products with the important property that the left- and the right-handed J -adjoint matrices are the same for all matrices A (see [15, Section 2.1.]), and can be expressed as $J^{-1} A^* J$, where A^* denotes the standard conjugate transpose of A . Then, a matrix S is J -selfadjoint or J -Hermitian, if

$$(1.6) \quad S = J^{-1} S^* J.$$

Similarly to the Euclidean case, we can define matrices Q that are unitary with respect to a given orthosymmetric J , as matrices that preserve the scalar product, i.e., $[Qx, Qy] = [x, y]$, for all $x, y \in \mathbb{F}^n$. In other words, Q is a J -unitary matrix if it satisfies

$$(1.7) \quad Q^* J Q = J.$$

Due to the defining preservation property, J -unitary matrices are essential tools in structure preserving algorithms. It is easy to see that J -unitary matrices form a multiplicative group. Therefore, they are usually represented and computed as a product of a sequence of J -unitary matrices with a simpler structure, resembling ordinary rotations and reflectors.

A hierarchical design of memory (frequently in multiple cache levels) in modern computing machinery enables programmers to write faster programs if the algorithms are properly blocked. Besides rotations and reflectors, such algorithms also require their blocked counterparts—block rotations and block reflectors. Moreover, some algorithms, like the symplectic QR factorization [14], cannot be constructed without the use of block transformations.

The mathematical background of ordinary block reflectors and the methods for their computation are given by Schreiber and Parlett in [12]. The construction of orthosymmetric block reflectors, with their mapping and annihilation properties, is given in [15]. The same construction, but restricted to the symplectic scalar product generated by (1.3) is given in [11], with an application to the symplectic block QR factorization.

For unknown reasons, the block rotations have been investigated far less than the block reflectors. The first traces of the representation of block rotations can be found in an unpublished manuscript attributed to Zakrajšek and Vidav [20]. Elementary matrices introduced by Veselić [19] can also be viewed as the indefinite block rotations. They are useful tools in the construction of the hyperbolic QR factorization [13].

Here, we extend the results of Zakrajšek and Vidav to matrices that are J -unitary with respect to an orthosymmetric scalar product. The main decomposition results are given in Section 2, while Section 3 deals with some computational aspects of block rotations, including possible applications in computing the QR-like factorization of a matrix, for some orthosymmetric scalar products.

2. Decomposition of J -unitary block matrices. In this section, we will decompose a J -unitary block matrix into a product of two simple J -unitary matrices. To this end, we need a few preparatory results, already known in the literature, but we state them here for completeness.

LEMMA 2.1. *Let $A \in \mathbb{C}^{m \times n}$ and $B \in \mathbb{C}^{n \times m}$ be given matrices, and let f be a function defined on the spectra of both AB and BA . Then*

$$Af(BA) = f(AB)A.$$

The proof can be found in [5, Corollary 1.34.].

In what follows, this lemma will mostly be used with the function f equal to the principal square root of a matrix, or its inverse. Let $A \in \mathbb{C}^{n \times n}$ be a matrix that

- (a) has no negative real eigenvalues, or
- (b) if zero is an eigenvalue of A , then it is semisimple.

Then there is a unique square root Z of A , whose nonzero eigenvalues lie in the open right half-plane [5, Section 1.7]. This unique square root is called the principal square

root of A and will be denoted by $A^{1/2}$. Its inverse is well-defined if A is nonsingular.

We will also need the notion of the generalized polar decomposition from [6]. In our terms, it is defined as follows.

DEFINITION 2.2. Given a scalar product generated by J on $\mathbb{F}^n$ as in (1.2), a *generalized polar decomposition* of $A \in \mathbb{F}^{n \times n}$ is a decomposition $A = WS$, where W is J -unitary, and S is J -Hermitian whose nonzero eigenvalues are contained in the open right half-plane.

If the underlying scalar product is orthosymmetric, i.e., J satisfies (1.1), then the following theorem [6, Theorem 2.7] holds.

THEOREM 2.3 (Generalized polar decomposition with unique selfadjoint factor). *Given an orthosymmetric scalar product defined by $J \in \mathbb{F}^{n \times n}$, a matrix $A \in \mathbb{F}^{n \times n}$ has a generalized polar decomposition $A = WS$ with a unique J -Hermitian factor S , if and only if the following three conditions are simultaneously satisfied*

- (a) $J^{-1}A^*JA$ has no negative real eigenvalues;
- (b) if zero is an eigenvalue of $J^{-1}A^*JA$, then it is semisimple; and
- (c) $\mathcal{N}(J^{-1}A^*JA) = \mathcal{N}(A)$, where $\mathcal{N}(A)$ denotes the nullspace of A , or equivalently, A is nondegenerate with respect to J (see [15, Proposition 2.2.]).

Now, suppose that a given matrix J of the orthosymmetric scalar product from (1.1) is block-diagonal, partitioned as

$$(2.1) \quad J = \text{diag}(J_1, J_2),$$

where $J_1 \in \mathbb{F}^{m \times m}$ and $J_2 \in \mathbb{F}^{(n-m) \times (n-m)}$, for some m such that $0 < m < n$.

The main result of this section states that, under mild conditions, a J -unitary matrix Q can be decomposed as a product of two simple J -unitary matrices, a block-diagonal matrix W and a block rotation U .

THEOREM 2.4. *Let J be a matrix of the orthosymmetric scalar product partitioned as in (2.1), and let Q be a J -unitary matrix with respect to J , partitioned in the same way as J ,*

$$(2.2) \quad Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}, \quad Q_{11} \in \mathbb{F}^{m \times m}, \quad Q_{22} \in \mathbb{F}^{(n-m) \times (n-m)}.$$

If the diagonal blocks Q_{11} and Q_{22} are nonsingular matrices that have the generalized polar decomposition (with regard to J_1 and J_2 , respectively), then Q from (2.2) can be factored as $Q = WU$, where W and U are J -unitary matrices, and

$$(2.3) \quad W = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix}, \quad U = \begin{bmatrix} (I - J_1^{-1}X^*J_2X)^{1/2} & -J_1^{-1}X^*J_2 \\ X & (I - XJ_1^{-1}X^*J_2)^{1/2} \end{bmatrix},$$

with $W_{11} \in \mathbb{F}^{m \times m}$, $W_{22} \in \mathbb{F}^{(n-m) \times (n-m)}$, and $X \in \mathbb{F}^{(n-m) \times m}$. Moreover, if the decomposition (2.3) exists, the diagonal blocks Q_{11} and Q_{22} have the generalized polar decomposition, with regard to J_1 and J_2 , respectively.

Proof. Suppose that, for $i = 1, 2$, the matrices Q_{ii} permit the generalized polar decomposition, i.e., there exist J_i -unitary matrices W_{ii} , and unique J_i -Hermitian matrices U_{ii} , such that

$$Q_{ii} = W_{ii}U_{ii}.$$

Then, Q from (2.2) can be written as

$$\begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} := WU = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}.$$

From the block-diagonal structure of J and W , it is obvious that W is a J -unitary matrix. Since J -unitary matrices form a multiplicative group, and $U = W^{-1}Q$, it follows that U is also J -unitary and, thus nonsingular. From (1.7), the blocks of U satisfy the following set of equations

$$(2.4) \quad U_{11}^* J_1 U_{11} + U_{21}^* J_2 U_{21} = J_1$$

$$(2.5) \quad U_{11}^* J_1 U_{12} + U_{21}^* J_2 U_{22} = 0$$

$$(2.6) \quad U_{12}^* J_1 U_{12} + U_{22}^* J_2 U_{22} = J_2.$$

Moreover, by inversion of $U^*JU = J$, we obtain $UJ^{-1}U^* = J^{-1}$, which means that U^* is J^{-1} -unitary, and the corresponding three block-equations are

$$(2.7) \quad U_{11} J_1^{-1} U_{11}^* + U_{12} J_2^{-1} U_{12}^* = J_1^{-1}$$

$$(2.8) \quad U_{11} J_1^{-1} U_{21}^* + U_{12} J_2^{-1} U_{22}^* = 0$$

$$(2.9) \quad U_{21} J_1^{-1} U_{21}^* + U_{22} J_2^{-1} U_{22}^* = J_2^{-1}.$$

We will show that the equations (2.4)–(2.9) can be solved in terms of a single matrix X , where $X = U_{21}$.

By multiplication of (2.4) from the left by J_1^{-1} we obtain

$$J_1^{-1} U_{11}^* J_1 U_{11} = I - J_1^{-1} X^* J_2 X.$$

Since U_{11} is J_1 -Hermitian, from (1.6) we get $U_{11}^* J_1 = J_1 U_{11}$, and the previous equality becomes

$$U_{11}^2 = I - J_1^{-1} X^* J_2 X.$$

By assumption, the block Q_{11} has the generalized polar decomposition $Q_{11} = W_{11}U_{11}$ with a unique J -Hermitian factor U_{11} , so $J_1^{-1}Q_{11}^*J_1Q_{11}$ can be written as

$$J_1^{-1}Q_{11}^*J_1Q_{11} = J_1^{-1}U_{11}^*(W_{11}^*J_1W_{11})U_{11} = (J_1^{-1}U_{11}^*J_1)U_{11} = U_{11}^2.$$

Then the three conditions that guarantee the existence of the generalized polar factor, yield that U_{11}^2 has a unique principal square root whose nonzero eigenvalues are contained in the open right half-plane. Since U_{11} satisfies this spectrum condition, we conclude that

$$(2.10) \quad U_{11} = (I - J_1^{-1}X^*J_2X)^{1/2}.$$

If the equation (2.9) is multiplied from the right by J_2 , a similar argument gives the principal square root

$$(2.11) \quad U_{22} = (I - XJ_1^{-1}X^*J_2)^{1/2}.$$

Now we use the fact that the matrix J in (2.1) is orthosymmetric, and (1.1) implies $J_1^{-*} = \tau^{-1}J_1^{-1}$ and $J_2^* = \tau J_2$. By substitution of (2.10) and (2.11) into (2.5), we obtain

$$(I - X^*J_2XJ_1^{-1})^{1/2}J_1U_{12} + X^*J_2(I - XJ_1^{-1}X^*J_2)^{1/2} = 0.$$

Finally, if we take $A = X^*J_2$, $B = XJ_1^{-1}$ and f as the principal square root in Lemma 2.1, we obtain

$$(I - X^*J_2XJ_1^{-1})^{1/2}J_1U_{12} = -(I - X^*J_2XJ_1^{-1})^{1/2}X^*J_2,$$

or, by using (2.10),

$$(2.12) \quad U_{11}^*J_1(U_{12} + J_1^{-1}X^*J_2) = 0.$$

If U_{11}^* is nonsingular, $U_{12} = -J_1^{-1}X^*J_2$ is a unique solution of (2.12).

Now suppose that the decomposition $Q = WU$, where W and U are defined by (2.3), is given. Since U_{ii} for $i = 1, 2$, is the principal square root, then U_{ii}^2 has no negative real eigenvalues, and if zero is an eigenvalue, it is semisimple. We have already shown that

$$U_{ii}^2 = J_i^{-1}Q_{ii}^*J_iQ_{ii}, \quad i = 1, 2,$$

i.e., we have proved the first two requirements for existence of the generalized polar decomposition of Q_{ii} . Finally, since the principal square root is a primary matrix function, we have $\mathcal{N}(U_{ii}^2) = \mathcal{N}(U_{ii})$, and thus

$$\mathcal{N}(J_i^{-1}Q_{ii}^*J_iQ_{ii}) = \mathcal{N}(U_{ii}^2) = \mathcal{N}(U_{ii}) = \mathcal{N}(W_{ii}U_{ii}) = \mathcal{N}(Q_{ii}),$$

that is the last requirement needed in Theorem 2.3 for the existence of the generalized polar decomposition with a unique J -Hermitian factor. $\square$

The equations (2.4)–(2.9) can also be solved in terms of $Y = U_{12}$, and then the blocks of U in (2.3) are all expressed in terms of Y . Since X and Y are simply connected by $Y = -J_1^{-1}X^*J_2$ (as noticed by Veselić [19] in the Euclidean and hyperbolic cases), the form of U in terms of Y follows easily.

Note that if Q and J are real matrices, then W and U are also real, because the same is valid for the principal square root and the generalized polar decomposition.

If Q_{11} in Theorem 2.4 is singular, a difficulty occurs in (2.12), since U_{11} is singular. In some special cases, Theorem 2.4 holds even for singular Q_{11} and Q_{22} .

PROPOSITION 2.5. *Let J be a matrix of the orthosymmetric scalar product partitioned as in (2.1), and let Q be a J -unitary matrix with respect to J , partitioned in the same way as J ,*

$$(2.13) \quad Q = \begin{bmatrix} 0 & Q_{12} \\ Q_{21} & 0 \end{bmatrix}, \quad Q_{12}, Q_{21} \in \mathbb{F}^{m \times m}.$$

then Q from (2.13) can be factored as $Q = WU$, where W and U are J -unitary matrices, and

$$W = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix}, \quad U = \begin{bmatrix} 0 & -J_1^{-1}X^*J_2 \\ X & 0 \end{bmatrix},$$

with $W_{11}, W_{22}, X \in \mathbb{F}^{m \times m}$.

Proof. First note that the diagonal blocks should be of the same size, and the off-diagonal blocks should be nonsingular. Otherwise, Q is singular, and thus cannot be J -orthogonal.

Note that $Q_{ii} = 0$, for $i = 1, 2$ have the generalized polar decomposition with the unique $U_{ii} = 0$. Since Q is J -unitary, the off-diagonal blocks satisfy

$$(2.14) \quad Q_{12}^* J_1 Q_{12} = J_2, \quad Q_{21}^* J_2 Q_{21} = J_1.$$

Let $W_{22} = I$, $U_{21} = X$ and $U_{12} = -J_1^{-1}X^*J_2$. It rests to prove that W_{11} , which satisfies

$$(2.15) \quad Q_{12} = W_{11}U_{12} = -W_{11}J_1^{-1}X^*J_2,$$

is J_1 -unitary. From (2.15) it follows $W_{11} = -Q_{12}J_2^{-1}X^*J_1$, which, together with (2.14) gives

$$(2.16) \quad W_1^* J_1 W_1 = J_1 X^{-1} J_2^{-1} (Q_{12} J_1 Q_{12}^*) J_2^{-1} X^{-*} J_1 = J_1 X^{-1} J_2^{-1} X^{-*} J_1.$$

Since $Q_{21} = X$ is nonsingular, inversion of the second equation in (2.14) yields $X^{-1}J_2^{-1}X^{-*} = J_1^{-1}$. Insertion into (2.16) gives $W_1^* J_1 W_1 = J_1$, which completes the proof. $\square$

If Q_{ii} , $i = 1, 2$, are singular, but not identically equal to zero, factorization (2.3) may still exist.

EXAMPLE 2.6. Suppose that

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix}, \quad Q_{11} = Q_{22} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad Q_{12} = Q_{21} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

while $J = \text{diag}(J_1, J_2)$, with $J_1 = J_2 = \text{diag}(-1, 1)$.

The matrices Q_{ii} have the generalized polar decompositions with unique U_{ii} ,

$$Q_{ii} = W_{ii} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad W_{ii} = \text{diag}(\pm 1, 0).$$

For chosen $W_{22} = I$, we obtain $X = U_{21} = Q_{21}$, and

$$U_{12} = -J_1^{-1} X^* J_2 = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix}.$$

It is easy to show that $W_{11} = \text{diag}(-1, 1)$ is J_1 -unitary and satisfies $Q_{1j} = W_{11} U_{1j}$, for $j = 1, 2$, so Q can be written as in (2.3).

In practice, the inverse and/or the conjugate transpose of Q is frequently required, as well. From (1.7) it follows that

$$Q^{-1} = J^{-1} Q^* J.$$

In the product representation $Q = WU$ from Theorem 2.4, the inverses and the conjugate transposes of both factors are easy to compute.

PROPOSITION 2.7. *Let W and U be the J -unitary factors of Q from (2.3). Then*

$$W^* = \text{diag}(W_{11}^*, W_{11}^*), \quad W^{-1} = \text{diag}(J_1^{-1} W_{11}^* J_1, J_2^{-1} W_{22}^* J_2),$$

the conjugate transpose of U is given by

$$U^* = \begin{bmatrix} (I - X^* J_2 X J_1^{-1})^{1/2} & X^* \\ -J_2 X J_1^{-1} & (I - J_2 X J_1^{-1} X^*)^{1/2} \end{bmatrix},$$

while the inverse of U is given by

$$(2.17) \quad U^{-1} = \begin{bmatrix} (I - J_1^{-1} X^* J_2 X)^{1/2} & J_1^{-1} X^* J_2 \\ -X & (I - X J_1^{-1} X^* J_2)^{1/2} \end{bmatrix}.$$

When $\mathbb{F} = \mathbb{R}$ and $n = 2$ (then $m = 1$), the only orthosymmetric scalar product matrices J satisfying (2.1) are

$$J_T = \pm \text{diag}(1, 1), \quad J_H = \pm \text{diag}(1, -1).$$

The corresponding matrices U from (2.3) can be written as

$$U_T = \begin{bmatrix} (1-x^2)^{1/2} & -x \\ x & (1-x^2)^{1/2} \end{bmatrix}, \quad U_H = \begin{bmatrix} (1+x^2)^{1/2} & x \\ x & (1+x^2)^{1/2} \end{bmatrix}.$$

By putting $x = \sin \varphi$ in U_T (since, obviously, $|x| \leq 1$), and $x = \sinh \varphi$ in U_H , we get the standard form of trigonometric and hyperbolic plane rotations

$$U_T = \begin{bmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{bmatrix}, \quad U_H = \begin{bmatrix} \cosh \varphi & \sinh \varphi \\ \sinh \varphi & \cosh \varphi \end{bmatrix}.$$

If the order of U is greater than 2, the blocks of U in (2.3) can be interpreted as block cosines and block sines by the following definition

$$(2.18) \quad U := \begin{bmatrix} C_1 & -S_2 \\ S_1 & C_2 \end{bmatrix} = \begin{bmatrix} (I - J_1^{-1} X^* J_2 X)^{1/2} & -J_1^{-1} X^* J_2 \\ X & (I - X J_1^{-1} X^* J_2)^{1/2} \end{bmatrix}.$$

Then it easy to verify that $C_1^2 + S_2 S_1 = I_m$ and $C_2^2 + S_1 S_2 = I_{n-m}$. Together with $S_2 = J_1^{-1} S_1^* J_2$, this structure of U justifies the term *block rotation*.

PROPOSITION 2.8. *Matrices C_1 and C_2 are either simultaneously singular, or simultaneously nonsingular.*

Proof. The Jordan structure associated with nonzero eigenvalues of $S_1 S_2$ and $S_2 S_1$ is identical (for the proof of this fact see [4, 18]). Especially, the Jordan structure for the eigenvalue 1 is identical. Therefore,

$$C_1^2 = I_m - S_2 S_1, \quad C_2^2 = I_{n-m} - S_1 S_2,$$

are either simultaneously singular, or simultaneously nonsingular. The same holds for their principal square roots C_1 and C_2 . $\square$

Since C_1 and C_2 can have different dimensions, we define four matrices that could serve as block tangents. As in the pointwise case, the tangents are undefined if C_1 and C_2 are singular. From now on, unless stated otherwise, we assume that the diagonal blocks C_1, C_2 of U are nonsingular.

DEFINITION 2.9. Let U be defined by (2.18) with nonsingular diagonal blocks. The corresponding four matrix *tangent* functions (of X) are defined by

$$(2.19) \quad T := S_1 C_1^{-1} = X(I - J_1^{-1} X^* J_2 X)^{-1/2},$$

$$(2.20) \quad \widehat{T} := S_2 C_2^{-1} = J_1^{-1} X^* J_2 (I - X J_1^{-1} X^* J_2)^{-1/2},$$

$$(2.21) \quad \widehat{T}_0 := C_1^{-1} S_2 = (I - J_1^{-1} X^* J_2 X)^{-1/2} J_1^{-1} X^* J_2,$$

$$(2.22) \quad T_0 := C_2^{-1} S_1 = (I - X J_1^{-1} X^* J_2)^{-1/2} X.$$

As can be expected, these four tangents are not independent. In fact, they are related in exactly the same way as the corresponding sines used in their definition.

PROPOSITION 2.10. *The matrix tangents defined by (2.19)–(2.22) are pairwise mutually equal, $T = T_0$, and $\hat{T} = \hat{T}_0$. Moreover, these pairs are connected by*

$$(2.23) \quad \hat{T} = J_1^{-1} T^* J_2,$$

in accordance with $S_2 = J_1^{-1} S_1^ J_2$.*

Proof. Consider the matrix T defined by (2.19). By using $A = X$, $B = J_1^{-1} X^* J_2$, and f as the inverse of the principal square root in Lemma 2.1, we have

$$T = X(I - J_1^{-1} X^* J_2 X)^{-1/2} = (I - X J_1^{-1} X^* J_2)^{-1/2} X = T_0.$$

The proof of the second equality is similar. By using Lemma 2.1 with $A = J_2$ and $B = X J_1^{-1} X^*$, we have

$$\hat{T} = J_1^{-1} X^* J_2 (I - X J_1^{-1} X^* J_2)^{-1/2} = J_1^{-1} X^* (I - J_2 X J_1^{-1} X^*)^{-1/2} J_2 = J_1^{-1} T^* J_2,$$

which completes the proof. $\square$

The ordinary plane rotations are frequently used in one-sided and two-sided matrix algorithms to annihilate a certain element of a given working matrix. In most cases, it is the *tangent* of an angle that is the easiest to calculate from the annihilation equation. The elements of the rotation matrix (i.e., the cosines and the sines) are then computed from the tangent.

The same is true for the block rotations, as will be demonstrated in the next section. We already know how to compute all the blocks of U once we have X (provided that the diagonal blocks are nonsingular and the principal square roots exist), so only X will have to be computed from the block tangent.

PROPOSITION 2.11. *If the tangent functions (2.19)–(2.22) exist, the matrix X from (2.3) can be expressed in terms of the tangent functions in several ways*

$$(2.24) \quad \begin{aligned} X &= (I + T\hat{T})^{-1/2} T = (I + T J_1^{-1} T^* J_2)^{-1/2} T \\ &= T(I + \hat{T}T)^{-1/2} = T(I + J_1^{-1} T^* J_2 T)^{-1/2}. \end{aligned}$$

Proof. From (2.22) for $T = T_0$ and (2.20) for $\hat{T}$, it follows

$$I + T\hat{T} = I + (I - X J_1^{-1} X^* J_2)^{-1/2} X J_1^{-1} X^* J_2 (I - X J_1^{-1} X^* J_2)^{-1/2}.$$

If we substitute $Z = X J_1^{-1} X^* J_2$, this can be written as

$$\begin{aligned} I + T\hat{T} &= I + (I - Z)^{-1/2} Z (I - Z)^{-1/2} \\ &= (I - Z)^{-1/2} ((I - Z) + Z) (I - Z)^{-1/2} = (I - Z)^{-1}. \end{aligned}$$

From (2.11) we see that $I - Z = U_{22}^2 = C_2^2$, so $I - Z$ has the principal square root,

$$(I - Z)^{1/2} = (I + T\hat{T})^{-1/2} = (I - XJ_1X^*J_2)^{1/2}.$$

A multiplication from the right by $T = T_0$ from (2.22) gives

$$(I + T\hat{T})^{-1/2}T = (I - XJ_1X^*J_2)^{1/2}(I - XJ_1^{-1}X^*J_2)^{-1/2}X = X.$$

This proves the first equality in (2.24). The second one follows by substitution of $\hat{T}$ from (2.23). Finally, the last two equalities are obtained from the first row in (2.24) by an obvious application of Lemma 2.1. $\square$

To conclude this section, note that the transformations $X \mapsto T$ and $T \mapsto X$ are the same, except for the sign under the square root

$$X \mapsto T = (I - XJ_1^{-1}X^*J_2)^{-1/2}X, \quad T \mapsto X = (I + TJ_1^{-1}T^*J_2)^{-1/2}T,$$

which greatly simplifies the computation.

Some caution is necessary before applying these transformations. If we know that U exists and X is given, then T is always well-defined (computable). On the other hand, if T is given, this does not automatically imply that X is well-defined by (2.24).

PROPOSITION 2.12. *If $T \in \mathbb{F}^{(n-m) \times m}$ is given, and X is well-defined by (2.24), then C_1 and C_2 in (2.18) are also well-defined.*

Proof. If T is given, then the matrix X is well-defined by (2.24) if and only if both $Z_1 := I + J_1^{-1}T^*J_2T$ and $Z_2 := I + TJ_1^{-1}T^*J_2$ have no negative or zero eigenvalues.

To show that C_1 is well-defined in (2.16), consider the matrix $I - J_1^{-1}X^*J_2X$. By using both equalities from (2.24) and Lemma 2.1 we have

$$\begin{aligned} I - J_1^{-1}X^*J_2X &= I - J_1^{-1}T^*(I + J_2TJ_1^{-1}T^*)^{-1/2}J_2T(I + J_1^{-1}T^*J_2T)^{-1/2} \\ &= I - J_1^{-1}T^*J_2T(I + J_1^{-1}T^*J_2T)^{-1} = I - (Z_1 - I)Z_1^{-1} = Z_1^{-1}. \end{aligned}$$

Since Z_1 has no negative or zero eigenvalues, the same holds for Z_1^{-1} , so the principal square root of Z_1^{-1} is well-defined and then $C_1 = Z_1^{-1/2}$.

The proof for C_2 is similar, as we get $C_2 = Z_2^{-1/2}$. Finally, note that if T is square and nonsingular, then Z_1 and Z_2 are similar, so it is sufficient to verify that one of the cosine blocks is well-defined. If so, then they are also similar. $\square$

Therefore, if T is given, only the existence of the inverse of the principal square roots in (2.3) has to be checked.

3. Applications. A typical application of the J -unitary block matrices W and U lies in the systematic annihilation of relatively small block matrices, either for

(one-sided) Givens-like QR factorization, or for two-sided block diagonalization by similarity or congruence transformations.

In these algorithms, the inverse or the conjugate transpose of Q is usually applied from the *left*-hand side to the working matrix, and (if needed) Q itself is used from the right-hand side. Since $Q = WU$, this means that W^* or W^{-1} is first applied from the left, followed by U^* or U^{-1} . The purpose of the block-diagonal matrix W^* or W^{-1} is to *prepare* the chosen blocks of the working matrix for the “actual” transformation (like annihilation) by the block rotation U^* or U^{-1} .

For the best part of this section, we will consider one-sided transformations in the QR-like factorizations with respect to some of the most frequently used orthosymmetric scalar products, and two-sided congruence transformations are illustrated in the last subsection. In all examples below, J will be a unitary matrix.

3.1. Euclidean scalar product. Let J in (2.1) be the Euclidean scalar product, with $J_1 = I_m$ and $J_2 = I_{n-m}$, or $J_1 = -I_m$ and $J_2 = -I_{n-m}$. In this case, we are dealing with the ordinary unitary block matrices.

Let Q be a unitary matrix partitioned as in (2.2). Zakrajšek and Vidav [20] showed that Q can always be decomposed as in (2.3), even if the diagonal blocks of Q are singular. This decomposition of Q is

$$(3.1) \quad Q = WU = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix} \begin{bmatrix} (I - X^*X)^{1/2} & -X^* \\ X & (I - XX^*)^{1/2} \end{bmatrix},$$

with unitary W and U . In this case, the relation between X and T from (2.24), if T exists, simplifies to

$$(3.2) \quad X = (I + TT^*)^{-1/2}T = T(I + T^*T)^{-1/2}.$$

If X has at least one singular value equal to 1, then U has singular diagonal blocks and T is nonexistent.

Now we will show that for any given T , the matrix X is well-defined by (3.2). Then, by Proposition 2.12, C_1 and C_2 are also well-defined by X , and it is easy to prove by using the SVD (the Singular Value Decomposition) of X , that they are Hermitian and positive definite, as well.

THEOREM 3.1. *If $T \in \mathbb{F}^{(n-m) \times m}$ is given, then X is well-defined by (3.2), and the matrices $I - X^*X$ and $I - XX^*$ are Hermitian and positive definite.*

For the ordinary plane rotations, this result simply says that for any value of $t = \tan \varphi$, we can compute $x = \sin \varphi$. On the other hand, if we start from a given value of x , and try to compute t , or any other element of U_T , then we must ensure that $|x| < 1$ (otherwise t is not defined), and the corresponding tangent t must exist.

An analogue of this fact for block rotations is the following “test matrix generation” problem: starting from a given matrix $X \in \mathbb{F}^{(n-m) \times m}$, we want to generate the block rotation U as in (3.1). To succeed, C_1 and C_2 have to be well-defined, and this is so if and only if all singular values of X are strictly less than 1 (see [19]). As we will see, in the hyperbolic case, the situation between X and T in that respect is exactly the opposite.

The block rotations U from (3.1) can be used for block annihilation in the computation of the QR factorization in a tree-like manner, by a divide-and-conquer algorithm, suitable for parallel computing.

EXAMPLE 3.2. Suppose that a matrix $G \in \mathbb{F}^{n \times k}$ is given, with $n \geq k$. Let $G^{(1)}$ be a submatrix of G that consists of the first m columns of G , where $m \leq k$ and $m < n$. If $G^{(1)}$ has the full column rank, there exists a nonsingular square submatrix G_1 (of order m) of $G^{(1)}$. By row permutations, this square submatrix can be brought to the top of $G^{(1)}$. The submatrix G_2 then contains the remaining rows of $G^{(1)}$.

Our goal is to annihilate the whole block G_2 , by using the inverse of the block rotation U from (3.1), partitioned in the same way as $G^{(1)}$. By using (2.17), the wanted transformation is

$$U^{-1}G^{(1)} = \begin{bmatrix} (I - X^*X)^{1/2} & X^* \\ -X & (I - XX^*)^{1/2} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \end{bmatrix} = \begin{bmatrix} G'_1 \\ 0 \end{bmatrix}.$$

The matrix $X \in \mathbb{F}^{(n-m) \times m}$ has to be determined from the second block equation, which is the annihilation equation

$$-XG_1 + (I - XX^*)^{1/2}G_2 = 0.$$

From here we obtain the matrix tangent

$$T = (I - XX^*)^{-1/2}X = G_2G_1^{-1},$$

which can be computed as a solution of the linear system $G_1T = G_2$, with multiple right-hand sides G_2 .

Once we have T , by Theorem 3.1, X and U are well-defined, and the square roots in U^{-1} can be computed by one of the methods described in [5, Chapter 6].

After the application of U^{-1} to the whole G , the new “working” matrix is

$$G' = U^{-1}G = \begin{bmatrix} G'_1 & G'_{12} \\ 0 & G'_{22} \end{bmatrix}.$$

In the next step, we can simultaneously transform the matrices G'_1 and G'_{22} . In each of the subsequent steps the number of independent transformations is doubled. The process finishes when all the square diagonal blocks become upper triangular.

Note that the preprocessing of blocks G_1 and G_2 by W_1^{-1} and W_2^{-1} , respectively, is not necessary here.

3.2. Hyperbolic scalar products. Now, let J in (2.1) be the hyperbolic scalar product in the standard partitioned form, with $J_1 = I_m$ and $J_2 = -I_{n-m}$, or $J_1 = -I_m$ and $J_2 = I_{n-m}$.

Let Q be a J -unitary matrix partitioned as in (2.2). It is easy to see that the diagonal blocks Q_{ii} of Q are always nonsingular, and thus have the generalized polar decomposition, since $J_i = \pm I$. The decomposition of Q from Theorem 2.4 always exists, and it is given by

$$(3.3) \quad Q = WU = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix} \begin{bmatrix} (I + X^*X)^{1/2} & X^* \\ X & (I + XX^*)^{1/2} \end{bmatrix},$$

with J -unitary W and U . Since W is block-diagonal, it is also a unitary matrix. By using the same technique as in [20], Šego [17] showed that this decomposition exists for a permuted J , i.e., for $J = \text{diag}(\pm 1)$, even if the diagonal blocks of Q are singular. A similar, but not identical decomposition of J -unitary matrix Q as in (3.3), is used in [16], in the block Cholesky downdating problem.

The relation between X and T from (2.24) now becomes

$$(3.4) \quad X = (I - TT^*)^{-1/2}T = T(I - T^*T)^{-1/2}.$$

The J -unitary “test matrix generation” problem is always solvable. For any given $X \in \mathbb{F}^{(n-m) \times m}$, both matrices $I + X^*X$ and $I + XX^*$ are Hermitian and positive definite, their principal square roots exist, so U in (3.3) is well-defined.

On the other hand, if T is given, the square roots in (3.4) need not exist, and then X cannot be computed from T . By using the SVD of T , it is easy to prove the following theorem.

THEOREM 3.3. *Let $T \in \mathbb{F}^{(n-m) \times m}$ be a given matrix. Then X is well-defined by (3.4) if and only if all singular values of T are strictly less than 1.*

When $n = 2$, we get the well-known fact that the hyperbolic plane rotation U_H is well-defined by t , if and only if the computed value of $t = \tanh \varphi$ satisfies $|t| < 1$.

As a consequence of Theorem 3.3, the hyperbolic block rotations U from (3.3) have a very limited use for block annihilation in the hyperbolic QR factorization.

EXAMPLE 3.4. Let $G \in \mathbb{F}^{n \times k}$ be a given matrix, with $n \geq k$, and let $G^{(1)}$ be a submatrix of G that consists of the first m columns of G , where $m \leq k$ and $m < n$, as in Example 3.2.

If the topmost square submatrix G_1 of $G^{(1)}$ is nonsingular, we can try to annihilate the remaining block G_2 of $G^{(1)}$ by using the inverse of the block rotation U from (3.3), partitioned in the *same* way as $G^{(1)}$,

$$U^{-1}G^{(1)} = \begin{bmatrix} (I + X^*X)^{1/2} & -X^* \\ -X & (I + XX^*)^{1/2} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \end{bmatrix} = \begin{bmatrix} G'_1 \\ 0 \end{bmatrix}.$$

The annihilation equation that determines X is

$$-XG_1 + (I + XX^*)^{1/2}G_2 = 0,$$

which gives the matrix tangent

$$T = (I + XX^*)^{-1/2}X = G_2G_1^{-1}.$$

By Theorem 3.3, the matrix X can be computed from this T , if and only if the singular values of $T = G_2G_1^{-1}$ are strictly less than 1, which is usually not the case.

If, by a stroke of luck, X is well-defined by T , then all subsequent transformations in a divide-and-conquer algorithm involve only ordinary unitary block rotations. Unfortunately, this “perfect splitting” rarely succeeds. Therefore, to compute the hyperbolic QR factorization, permutations of J have to be allowed, the working blocks have to be smaller (usually, of order 2), and often preprocessed to ensure the existence of J -unitary block transformations (see [13] for details).

3.3. Symplectic scalar products. Finally, let J in (2.1) be the symplectic scalar product of even order $n = 2p$, in the block-diagonal form (1.4). The matrix J can be partitioned as $J = \text{diag}(J_1, J_2)$ in several different ways, where the dimensions of J_1 and J_2 are also even, $m = 2q$ and $n - m = 2(p - q)$, respectively, but not necessarily the same. Both J_1 and J_2 inherit the inner structure from J , with possibly multiple copies of the block J_0 on their diagonal. In addition, since $J^{-1} = -J$, the same holds for the inverses of J_1 and J_2 .

Symplectic scalar products are usually considered over the real field $\mathbb{F} = \mathbb{R}$, and $n = 2p$ reflects the isomorphism of $\mathbb{C}^p$ and $\mathbb{R}^{2p}$. In that view, the symplectic scalar product J on $\mathbb{R}^{2p}$ corresponds to the “imaginary” orthosymmetric scalar product $J_c := iI_p$ on $\mathbb{C}^p$. To stress the fact that all matrices are real, in this subsection, we will use the ordinary transposes, instead of the conjugate transposes.

The following result for matrices of order 2 will be used subsequently in the construction of various examples.

LEMMA 3.5. *Let $Z \in \mathbb{R}^{2 \times 2}$ be a given matrix, and let J_0 be the elementary symplectic scalar product from (1.4). Then*

$$Z^T J_0 Z = (\det Z) J_0, \quad J_0 Z^T J_0 Z = Z J_0 Z^T J_0 = -(\det Z) I_2.$$

Proof. The first result follows by straightforward multiplication and the second one follows from $J_0^{-1} = J_0^T = -J_0$. $\square$

Let Q be a J -unitary matrix partitioned as in (2.2). Such a matrix satisfies $Q^T J Q = J$, and it is usually called a symplectic matrix. If the assumptions of Theorem 2.4 are fulfilled, the decomposition of Q has the following form

$$(3.5) \quad Q = WU = \begin{bmatrix} W_{11} & 0 \\ 0 & W_{22} \end{bmatrix} \begin{bmatrix} (I + J_1 X^T J_2 X)^{1/2} & J_1 X^T J_2 \\ X & (I + X J_1 X^T J_2)^{1/2} \end{bmatrix},$$

with symplectic W and U , and the relation between X and T from (2.24) becomes

$$(3.6) \quad X = (I - T J_1 T^T J_2)^{-1/2} T = T (I - J_1 T^T J_2 T)^{-1/2}.$$

In contrast to the previous two subsections, it is easy to construct an example of a diagonal block Q_{ii} that is nonsingular, but does not have the generalized polar decomposition. For example, let the blocks of Q in (2.2) be given by

$$Q_{11} = Q_{22} = \text{diag}(-1, 1), \quad Q_{12} = Q_{21} = \sqrt{2}I_2.$$

Then it is easy to verify that Q is symplectic, but the diagonal blocks have no generalized polar decomposition, since $J_0^{-1} Q_{ii}^T J_0 Q_{ii} = -I_2$, thus violating the condition (a) of Theorem 2.3. Therefore, one has to be careful to ensure the existence of (3.5).

Moreover, here it is not easy to determine in advance when the maps $X \mapsto T$ and $T \mapsto X$ are well-defined. A sufficient condition is provided by the following argument. Suppose that $Z \in \mathbb{R}^{(n-m) \times m}$ is given, where Z denotes either X or T . If the singular values σ_i of Z are strictly less than 1, the inverses of the principal square roots of the following four matrices $I \pm Z J_1 Z^T J_2$ and $I \pm J_1 Z^T J_2 Z$ exist. This follows from

$$\|Z J_1 Z^T J_2\|_2 \leq \|Z\|_2 \|J_1\|_2 \|Z^T\|_2 \|J_2\|_2 = \|Z\|_2 \|Z^T\|_2 = \sigma_{\max}^2(Z) < 1,$$

and similarly for $J_1 Z^T J_2 Z$, since J_1 and J_2 are unitary matrices. Hence, the spectra of both $Z J_1 Z^T J_2$ and $J_1 Z^T J_2 Z$ lie in the open unit circle, so $I \pm Z J_1 Z^T J_2$ and $I \pm J_1 Z^T J_2 Z$ have no negative or zero eigenvalues.

On the other hand, this condition is certainly not necessary. For example, let

$$T = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}.$$

The singular values of T are 3 and 1, but, by using Lemma 3.5, $I - T J_0 T^T J_0 = I - J_0 T^T J_0 T = 4I_2$, and the inverse of the principal square roots in (3.6) can be computed, giving $X = \frac{1}{2}T$.

We see that in the symplectic case, with arbitrary p and q , the “test matrix generation” problem is not easy to solve. Likewise, the general blocked version of the symplectic QR factorization encounters a similar problem as in the hyperbolic case—the required block rotation U does not have to be well-defined by the block tangent T determined from the annihilation equation, i.e., U may not exist.

From now on, we will consider the symplectic QR factorization (sometimes also called the SR factorization, as in [1]) only in the “minimal” nontrivial case $n = 4$ and $m = 2$. Then $J_1 = J_2 = J_0$. All the problems mentioned above will also appear here, but, as we will show, they can be solved by an adequate preprocessing of blocks.

To begin with, in this “minimal” case, it is easy to characterize when X is well-defined by T .

PROPOSITION 3.6. *Let $T \in \mathbb{R}^{2 \times 2}$ be a given matrix, and let $J_1 = J_2 = J_0$. Then X is well-defined by (3.6) if and only if $\det(T) > -1$.*

Proof. By using Lemma 3.5, we obtain

$$I - TJ_0T^TJ_0 = I - J_0T^TJ_0T = (1 + \det T)I_2.$$

Since $\det T$ is real, $(1 + \det T)I_2$ has positive eigenvalues if and only if $\det T > -1$. This means that X is computable from (3.6), and by Proposition 2.12, the whole block rotation U of order 4 in (3.5) is well-defined. $\square$

EXAMPLE 3.7. Let $J_1 = J_2 = J_0$ and we would like to obtain the symplectic QR factorization of a given matrix $G \in \mathbb{R}^{4 \times 2}$, with a nonsingular topmost block G_1 of order 2. The problem is to solve the following block equation in terms of X

$$U^{-1}G = \begin{bmatrix} (I + J_0X^TJ_0X)^{1/2} & -J_0X^TJ_0 \\ -X & (I + XJ_0X^TJ_0)^{1/2} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \end{bmatrix} = \begin{bmatrix} G'_1 \\ 0 \end{bmatrix}.$$

The annihilation equation that determines X is

$$-XG_1 + (I + XJ_0X^TJ_0)^{1/2}G_2 = 0,$$

which gives the matrix tangent

$$T = (I + XJ_0X^TJ_0)^{-1/2}X = G_2G_1^{-1}.$$

By Proposition 3.6, X is well-defined by T if and only if

$$-1 < \det(T) = \det(G_2G_1^{-1}) = \frac{\det(G_2)}{\det(G_1)}.$$

If G_2 is singular, then the previous inequality is always satisfied. On the other hand, if $\det(G_2)/\det(G_1) < -1$, then we can use a row permutation to swap the roles of

G_1 and G_2 , and obtain $\det(G_1)/\det(G_2) > -1$. Then $T = G_1 G_2^{-1}$ (in terms of the original blocks), so X is again well-defined by T .

Unfortunately, this row permutation will not help if $\det(G_1) = -\det(G_2)$. Then

$$I - T J_0 T^T J_0 = I - J_0 T^T J_0 T = 0,$$

and X is not computable.

Now suppose that $G \in \mathbb{R}^{4 \times 2}$ is preprocessed by a suitably chosen W^{-1} , where W is the block-diagonal factor from (3.5). It is easy to show that the ordinary unitary plane rotations are also J_0 -unitary matrices, and we can compute the QR factorization in each block G_i , i.e., we factorize $G_i = W_{ii} R_i$. This preprocessing gives a new working matrix $R \in \mathbb{R}^{4 \times 2}$ such that

$$R := \begin{bmatrix} W_{11}^{-1} & 0 \\ 0 & W_{22}^{-1} \end{bmatrix} \begin{bmatrix} G_1 \\ G_2 \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}, \quad R_1 = \begin{bmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{bmatrix}, \quad R_2 = \begin{bmatrix} r_{31} & r_{32} \\ 0 & r_{42} \end{bmatrix},$$

with positive diagonal elements in R_1 , and nonnegative in R_2 . The block rotation U from (3.5) is now used to annihilate the block R_2

$$U^{-1}R = \begin{bmatrix} (I + J_0 X^T J_0 X)^{1/2} & -J_0 X^T J_0 \\ -X & (I + X J_0 X^T J_0)^{1/2} \end{bmatrix} \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} = \begin{bmatrix} R'_1 \\ 0 \end{bmatrix},$$

which gives the upper triangular matrix tangent T

$$T = R_2 R_1^{-1} = \begin{bmatrix} \frac{r_{31}}{r_{11}} & \frac{r_{11}r_{32} - r_{12}r_{31}}{r_{11}r_{22}} \\ 0 & \frac{r_{42}}{r_{22}} \end{bmatrix}.$$

From the signs of the diagonal elements of R_1 and R_2 it follows that

$$\det(T) = \frac{\det(R_2)}{\det(R_1)} = \frac{r_{31}r_{42}}{r_{11}r_{22}} \geq 0,$$

and, by Proposition 3.6, X in (3.6) is always well-defined by T . Then we have

$$X = \frac{1}{\sqrt{1 + \det(T)}} T = \sqrt{\frac{r_{11}r_{22}}{r_{11}r_{22} + r_{31}r_{42}}} T,$$

and the whole block rotation U is given by

$$U^{-1} = \sqrt{\frac{r_{11}r_{22}}{r_{11}r_{22} + r_{31}r_{42}}} \begin{bmatrix} 1 & 0 & \frac{r_{42}}{r_{22}} & -\frac{r_{11}r_{32} - r_{12}r_{31}}{r_{11}r_{22}} \\ 0 & 1 & 0 & \frac{r_{31}}{r_{11}} \\ -\frac{r_{31}}{r_{11}} & -\frac{r_{11}r_{32} - r_{12}r_{31}}{r_{11}r_{22}} & 1 & 0 \\ 0 & -\frac{r_{42}}{r_{22}} & 0 & 1 \end{bmatrix}.$$

The result of this transformation is

$$U^{-1}R = \begin{bmatrix} R'_1 \\ 0 \end{bmatrix}, \quad R'_1 = \sqrt{1 + \det(T)} R_1 = \sqrt{1 + \frac{r_{31}r_{42}}{r_{11}r_{22}}} \begin{bmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{bmatrix}.$$

Note that the annihilation of R_2 preserves the upper triangular form of R_1 .

A systematic application of this procedure (annihilation of blocks of order 2, with preprocessing of blocks) gives a “non-blocked” version of the Givens-like algorithm for computing the symplectic QR factorization of a given matrix $G \in \mathbb{R}^{2p \times 2r}$ in the general case. The only condition is that in each step of the algorithm, there exists a nonsingular submatrix of order 2, corresponding to a block J_0 in J ,

$$\begin{bmatrix} g_{2i-1,2i-1} & g_{2i-1,2i} \\ g_{2i,2i-1} & g_{2i,2i} \end{bmatrix}$$

in the working part of the matrix. A similar algorithm for computing the symplectic QR factorization is given in [14]. The transformations used in that algorithm (see Lemma 2.2 therein) are given by

$$(3.7) \quad S_1 = U_T \otimes I_2 = \begin{bmatrix} \cos \varphi I_2 & -\sin \varphi I_2 \\ \sin \varphi I_2 & \cos \varphi I_2 \end{bmatrix}, \quad S_2 = \begin{bmatrix} I_2 & X_2 \\ X_2 & I_2 \end{bmatrix}, \quad X_2 = \begin{bmatrix} 0 & a \\ 0 & 0 \end{bmatrix},$$

and it is easy to verify that they are also symplectic block rotations.

In some applications, the symplectic QR factorization of G with symplectic and orthogonal $\hat{Q}$ has to be computed. Kressner [7] uses the Givens rotations and the orthogonal symplectic reflectors. If $J = P^T \hat{J} P$, as in (1.5), and $Q = P^T \hat{Q} P$, the same factorization can be achieved by using W and U from (3.5). The final R is the same as in [1, Corollary 4.5 (iii)] if $G \in \mathbb{R}^{2n \times 2n}$, or as in [7, Lemma 1.1] if $G \in \mathbb{R}^{2m \times 2n}$, $m \geq n$. A similar algorithm based on block rotations is essentially described in [14, Section 2.2.], if the applications of the nonunitary transformations S_2 from (3.7) are omitted in Step 5 of the algorithm.

3.4. Unitary block transformations of scalar products. An essential assumption in Theorem 2.4 and the whole construction of J -unitary block rotations is that a given orthosymmetric scalar product J satisfies (2.1), i.e., that it is block-diagonal.

Suppose that we have an orthosymmetric matrix $\hat{J}$ that is not block-diagonal. From (1.1) it is obvious that $\hat{J}$ is a normal matrix, so it can always be brought into a diagonal form by a unitary similarity (or congruence) transformation, i.e., there exists a unitary matrix $\hat{U}$ such that

$$\hat{U}^* \hat{J} \hat{U} = \text{diag}(j_1, \dots, j_n).$$

It is easy to verify that $J := \text{diag}(j_1, \dots, j_n)$ generates an orthosymmetric scalar product, with the same τ in (1.1) as $\hat{J}$. Now we can choose how to split J as in (2.1).

But, such a “drastic” diagonalization of $\hat{J}$ is not really necessary. It is quite sufficient to find a unitary similarity that transforms $\hat{J}$ into a block-diagonal J with only two diagonal blocks, as in (2.1). In some cases, this transformation can be accomplished easily by using unitary block rotations.

As an example, consider a Hermitian unitary matrix $\hat{J}$ with a block-antidiagonal structure. By using the SVD of J_0 (see for example [3, Theorem 3.3]) it is easy to prove the following result.

PROPOSITION 3.8. *Suppose that $\hat{J}$ has the following block structure*

$$\hat{J} = \begin{bmatrix} 0 & \hat{J}_0 \\ \hat{J}_0^* & 0 \end{bmatrix}$$

where $\hat{J}_0$ is a unitary matrix. There exists a unitary block rotation U ,

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -\hat{J}_0 \\ \hat{J}_0^* & I \end{bmatrix},$$

such that

$$U^* \hat{J} U = J = \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix}.$$

Moreover, $J_1 = I$ and $J_2 = -I$, so we get the hyperbolic scalar product.

Subsequently, we may use J -unitary matrices (including block rotations) in a structure preserving algorithm. If, for any reason, we need to reconstruct the transformations in the original scalar product $\hat{J}$, it is easy to do so by using U .

If Q is a J -unitary matrix, and $J = U^* \hat{J} U$, where U is a unitary matrix, then

$$(UQ^*U^*)\hat{J}(UQU^*) = UQ^*JQU^* = UJU^* = \hat{J},$$

which shows that $\hat{Q} := UQU^*$ is a $\hat{J}$ -unitary matrix.

4. Conclusion. In this paper, the orthosymmetric block rotations are introduced, and the potential applications are illustrated. Many QR-like factorization algorithms rely on orthosymmetric block rotations (or orthosymmetric block reflectors). The main application of block rotations given here, lies in the construction of relatively small orthosymmetric block rotations (e.g., of order 4), which—after preprocessing by W —do the annihilation job. The role of preprocessing by W is given only as a demonstration. Definitive answer how to preprocess a “big” block (of order

64, or even bigger) to ensure the existence of a block rotation that annihilates such a “big” block is a point for future research.

Acknowledgment. The author would like to thank Saša Singer for helpful comments on earlier versions of this paper. Many thanks to an anonymous referee for detailed and valuable comments which helped to improve the quality of this paper.

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