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THE CANONICAL GENERALIZED POLAR DECOMPOSITION*

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Abstract. The polar decomposition of a square matrix has been generalized by several authors to scalar products on \mathbb{R}^n or \mathbb{C}^n given by a bilinear or sesquilinear form. Previous work has focused mainly on the case of square matrices, sometimes with the assumption of a Hermitian scalar product. We introduce the canonical generalized polar decomposition $A = WS$, defined for general $m \times n$ matrices A , where W is a partial (M, N) -isometry and S is N -selfadjoint with nonzero eigenvalues lying in the open right half-plane, and the nonsingular matrices M and N define scalar products on \mathbb{C}^m and \mathbb{C}^n , respectively. We derive conditions under which a unique decomposition exists and show how to compute the decomposition by matrix iterations. Our treatment derives and exploits key properties of (M, N) -partial isometries and orthosymmetric pairs of scalar products, and also employs an appropriate generalized Moore–Penrose pseudoinverse. We relate commutativity of the factors in the canonical generalized polar decomposition to an appropriate definition of normality. We also consider a related generalized polar decomposition $A = WS$, defined only for square matrices A and in which W is an automorphism; we analyze its existence and the uniqueness of the selfadjoint factor when A is singular.

Key words. generalized polar decomposition, canonical polar decomposition, automorphism, selfadjoint matrix, bilinear form, sesquilinear form, scalar product, adjoint, orthosymmetric scalar product, partial isometry, pseudoinverse, matrix sign function, matrix square root, matrix iteration

AMS subject classifications. 15A23, 65F30,

1. Introduction. The polar decomposition is a much-studied matrix decomposition, from the points of view of both theory and computation. Depending on the matrix dimensions and the uniqueness required of the factors, it exists in several forms, of which we identify two. The first, defined for $A \in \mathbb{K}^{m \times n}$ with the restriction $m \geq n$, is described in the following theorem, where it is characterized in terms of the singular value decomposition (SVD). Here, \mathbb{K} denotes the field \mathbb{R} or \mathbb{C} , and for a matrix $A \in \mathbb{C}^{n \times n}$ having no eigenvalues on \mathbb{R}^- , the closed negative real axis, we denote by $A^{1/2}$ the principal square root, which is the unique square root all of whose eigenvalues lie in the open right half-plane [10, Sec. 1.7].

THEOREM 1.1 (polar decomposition [10, Thm. 8.1]). *For any $A \in \mathbb{K}^{m \times n}$ with $m \geq n$ there exists a matrix $U \in \mathbb{K}^{m \times n}$ with orthonormal columns and a unique Hermitian positive semidefinite matrix $H \in \mathbb{K}^{n \times n}$ such that $A = UH$. The matrix H is given by $(A^*A)^{1/2}$. All possible U are given by*

$$(1.1) \quad U = P \begin{bmatrix} I_r & 0 \\ 0 & W \end{bmatrix} Q^*,$$

where $A = P \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0_{m-r, n-r} \end{bmatrix} Q^*$ is an SVD, $r = \text{rank}(A)$, and $W \in \mathbb{K}^{(m-r) \times (n-r)}$ is arbitrary subject to having orthonormal columns.

The decomposition in Theorem 1.1 is unique if and only if A has full rank. The decomposition finds use in many applications, which often exploit the fact that U is a nearest matrix to A with orthonormal columns for any unitarily invariant norm [5], [10,

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Thm. 8.4]. An alternative decomposition, termed the canonical polar decomposition in [10], can be defined for all m and n in such a way that it is always unique. Recall that a matrix $U \in \mathbb{K}^{m \times n}$ is a partial isometry if $\|Ux\|_2 = \|x\|_2$ for all $x \in \text{range}(U^*)$, or equivalently, if $U^+ = U^*$, where U^+ denotes the Moore–Penrose pseudoinverse.

THEOREM 1.2 (canonical polar decomposition [10, Thm. 8.3]). *Any $A \in \mathbb{K}^{m \times n}$ has a unique decomposition $A = UH$ with $U \in \mathbb{K}^{m \times n}$ a partial isometry, $H \in \mathbb{K}^{n \times n}$ Hermitian positive semidefinite, and $\text{range}(U^*) = \text{range}(H)$. The factors U and H are given by $H = (A^*A)^{1/2}$ and $U = AH^+$. Moreover, $A^+ = H^+U^+$. Furthermore, if $A = P \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0_{m-r, n-r} \end{bmatrix} Q^*$ is an SVD then*

$$(1.2) \quad U = P \begin{bmatrix} I_r & 0 \\ 0 & 0_{m-r, n-r} \end{bmatrix} Q^*, \quad H = Q \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0_{n-r} \end{bmatrix} Q^*.$$

Our interest in this work is in a generalized polar decomposition $A = WS$ introduced for nonsingular square matrices by Higham, Mackey, Mackey, and Tisseur [12] in which W is an automorphism and S is selfadjoint with spectrum in the open right half-plane, where both properties are defined with respect to a general scalar product. Conditions that are both necessary and sufficient for the existence of this decomposition are identified in [12]. We investigate the following questions.

- What can be said about the existence and uniqueness of the generalized polar decomposition for (square) singular matrices, where S is now allowed to have zero eigenvalues?
- Can the canonical polar decomposition be extended to general scalar products, still for arbitrary rectangular matrices?
- Are there matrix iterations for computing the canonical polar decomposition, when the decomposition is unique?

We begin in section 2 by introducing the scalar product and associated terminology. We define the generalized polar decomposition $A = WS$ for an arbitrary square matrix A and obtain necessary conditions for a singular matrix to have such a decomposition, as well as necessary and sufficient conditions for a decomposition to exist with a unique selfadjoint factor S when the scalar product is orthosymmetric. The W factor is shown never to be unique in the singular case.

In section 3 we turn to rectangular matrices and define the canonical generalized polar decomposition $A = WS$, in which W is now a partial (M, N) -isometry, where M and N define the underlying scalar products. Under the assumption that the matrices M and N form what we call an orthosymmetric pair, we identify conditions under which the canonical generalized polar decomposition is unique. Our development makes use of an (M, N) -Moore–Penrose pseudoinverse A^\dagger and yields several useful relations that hold for orthosymmetric pairs, such as $A = WS \Rightarrow A^\dagger = S^\dagger W^\dagger$, which is a direct generalization of a relation in Theorem 1.2. In section 4 we obtain conditions for commutativity of the factors in the canonical generalized polar decomposition (assumed unique) in terms of an appropriate definition of normality, thereby generalizing the well-known fact that the usual polar factors commute if and only if A is normal. Computation of the canonical generalized polar decomposition by matrix iterations is considered in section 5, where we exploit a connection with the matrix sign function. Conclusions are given in section 6.

Aside from its theoretical interest this work has practical applications. Polar decompositions in scalar product spaces defined by indefinite Hermitian matrices enable the solution of corresponding Procrustes problems, as shown by Kintzel [17]. More-

over, a (canonical) generalized polar decomposition $A = WS$ along with a method for computing it provides a way of computing random automorphisms or partial isometries W from random A , as well as a means of “orthogonalizing” a matrix that has lost its property of being an automorphism or partial isometry, as discussed in [9] in the case of J -orthogonality.

Finally, we note some additional connections with earlier work. Kamaraj and Sivakumar [14] explore a generalization of the Moore–Penrose inverse to indefinite scalar product spaces; it is formally the same as our definition but throughout [14] the matrices of the inner product are assumed to be Hermitian. Yang and Li [22] explore a certain weighted generalized polar decomposition of rectangular matrices. It is defined only with respect to positive definite scalar products and does not reduce to our canonical generalized polar decomposition; in particular the definition of “ (M, N) weighted partial isometry” of [22] is different from our notion of partial (M, N) isometry when M or N is indefinite. In [1], [3], and [20] necessary and sufficient conditions are given for the existence of decompositions of the form $A = WS$, where W is an automorphism and S is selfadjoint with respect to a Hermitian sesquilinear form. These decompositions do not impose any restrictions on the spectrum of S . The decompositions that we study do constrain the spectrum of S but are less restrictive on the scalar product, essentially requiring only orthosymmetry.

2. Generalized polar decompositions. Consider a scalar product on \mathbb{K}^n defined in terms of a nonsingular matrix M by

$$(2.1) \quad \langle x, y \rangle_M = \begin{cases} x^T M y, & \text{for real or complex bilinear forms,} \\ x^* M y, & \text{for sesquilinear forms.} \end{cases}$$

With respect to this scalar product the following terminology is defined. The adjoint A^\star of $A \in \mathbb{K}^{n \times n}$ is the unique matrix satisfying $\langle Ax, y \rangle_M = \langle x, A^\star y \rangle_M$ for all $x, y \in \mathbb{K}^n$, and is given by

$$(2.2) \quad A^\star = \begin{cases} M^{-1} A^T M, & \text{for bilinear forms,} \\ M^{-1} A^* M, & \text{for sesquilinear forms.} \end{cases}$$

The matrix $A \in \mathbb{K}^{n \times n}$ is an automorphism if $A^\star = A^{-1}$ and is selfadjoint if $A^\star = A$.

All the results in this paper hold for both bilinear forms and sesquilinear forms. We will give the proofs only for sesquilinear forms and will comment on the differences (if any) in the proofs for bilinear case.

Higham, Mackey, and Tisseur [12, Sec. 4] define the generalized polar decomposition of a matrix $A \in \mathbb{K}^{n \times n}$ to be a decomposition $A = WS$, where W is an automorphism with respect to $\langle \cdot, \cdot \rangle_M$ and S is selfadjoint with spectrum contained in the open right half-plane. Clearly, such an S is nonsingular and thus A must be nonsingular in order to have a generalized polar decomposition. We now extend the notion of generalized polar decomposition to include singular matrices.

Throughout this section it is understood that the scalar product is (2.1). When we need to indicate the choice of M we will write “ M -generalized polar decomposition” or A^{\star_M} .

DEFINITION 2.1 (generalized polar decomposition). *Given a scalar product on \mathbb{K}^n , a generalized polar decomposition of $A \in \mathbb{K}^{n \times n}$ is a decomposition $A = WS$, where W is an automorphism and S is a selfadjoint matrix whose nonzero eigenvalues are contained in the open right half-plane, that is, $W^\star = W^{-1}$, $S^\star = S$, and $\Lambda(S) \subseteq \{z \in \mathbb{C} : \operatorname{Re}(z) > 0\} \cup \{0\}$.*

For the standard Euclidean scalar product $\langle x, y \rangle = x^*y$, the generalized polar decomposition is the usual polar decomposition $A = UH$, where U is unitary and H Hermitian positive semidefinite.

Existence and uniqueness of the generalized polar decomposition for nonsingular matrices is answered by the following result of Higham, Mackey, and Tisseur [12, Thm. 4.1] (see also [18, Thm. 6.2]).

THEOREM 2.2 (generalized polar decomposition of nonsingular matrices). *A nonsingular matrix $A \in \mathbb{K}^{n \times n}$ has a generalized polar decomposition $A = WS$ with respect to a scalar product on \mathbb{K}^n if and only if $(A^*)^* = A$ and A^*A has no eigenvalues on \mathbb{R}^- . When such a factorization exists it is unique.*

For the singular case the situation is more complicated. We begin by deriving three necessary conditions for existence.

THEOREM 2.3. *If $A \in \mathbb{K}^{n \times n}$ has a generalized polar decomposition $A = WS$ with respect to a scalar product on \mathbb{K}^n , then $(A^*)^* = A$, A^*A has no negative real eigenvalues, and S is a square root of A^*A .*

Proof. If the factorization exists then $(A^*)^* = (S^*W^*)^* = (SW^{-1})^* = W^{-*}S^* = WS = A$. The other conditions follow from $A^*A = S^*W^*WS = S^2$ and the spectral properties of S . \square

The first condition in Theorem 2.3 is satisfied if we restrict attention to the orthosymmetric scalar products introduced by Mackey, Mackey, and Tisseur [18], [19], which are those for which $(A^*)^* = A$ for all $A \in \mathbb{K}^{m \times m}$, that is, for which the adjoint is involutory. Many of the commonly used scalar products are orthosymmetric [18, Table 2.1]. Orthosymmetry can be characterized as follows [18, Thm. A.5].

THEOREM 2.4. *The scalar product $\langle \cdot, \cdot \rangle_M$ is orthosymmetric if and only if $M^T = \pm M$ for bilinear forms or $M^* = \alpha M$ with $\alpha \in \mathbb{C}$ and $|\alpha| = 1$ for sesquilinear forms.*

For an example (taken from [1], [3]) in which the necessary conditions of Theorem 2.3 do not all hold, consider

$$(2.3) \quad M = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and the matrix $A = \begin{bmatrix} 0 & 1 \\ 0 & \frac{1}{2} \end{bmatrix}$. We have

$$A^*A = \begin{bmatrix} \frac{1}{2} & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},$$

which does not have any square root, let alone a selfadjoint one.

For singular matrices, even when a generalized polar decomposition exists the selfadjoint factor need not be unique, as the following example illustrates. Consider again the scalar product induced by M in (2.3). Then

$$(2.4) \quad A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix}$$

are two generalized polar decompositions of A with different selfadjoint factors.

We now develop conditions for the existence of a generalized polar decomposition with a unique selfadjoint factor. The following lemmas will be exploited below.

LEMMA 2.5. *For any selfadjoint $S \in \mathbb{K}^{n \times n}$ with respect to a scalar product $\langle \cdot, \cdot \rangle_M$ on \mathbb{K}^n there exists a nonsingular matrix $X \in \mathbb{K}^{n \times n}$ such that*

$$X^{-1}SX = \begin{bmatrix} S_1 & 0 \\ 0 & S_0 \end{bmatrix}, \quad X^\#MX = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix},$$

where the partitionings are conformal and S_1 is nonsingular, S_0 is nilpotent, and $X^\# = X^T$ in the case of a bilinear form or $X^\# = X^*$ in the case of a sesquilinear form.

Proof. Let $X \in \mathbb{K}^{n \times n}$ be such that

$$X^{-1}SX = \begin{bmatrix} S_1 & 0 \\ 0 & S_0 \end{bmatrix}$$

is in Jordan canonical form (real Jordan canonical form when $\mathbb{K} = \mathbb{R}$) with S_1 nonsingular and S_0 nilpotent. For sesquilinear forms let

$$X^*MX = \begin{bmatrix} M_1 & M_2 \\ M_3 & M_0 \end{bmatrix},$$

where M_1 has the same size as S_1 . Then $S^\star = M^{-1}S^*M = S$ implies that

$$\begin{bmatrix} S_1^*M_1 & S_1^*M_2 \\ S_0^*M_3 & S_0^*M_0 \end{bmatrix} = X^*S^*MX = X^*MSX = \begin{bmatrix} M_1S_1 & M_2S_0 \\ M_3S_1 & M_0S_0 \end{bmatrix}.$$

The fact that the Sylvester equation $AY = YB$ has only the trivial solution $Y = 0$ if the spectra of A and B do not intersect implies that $M_2 = 0$ and $M_3 = 0$.

The proof for bilinear forms is analogous with conjugate transpose replaced by transpose. \square

The next lemma is a special case of Lemma 3.8 below (with $M = N$), so we omit the proof.

LEMMA 2.6. *For a given scalar product $\langle \cdot, \cdot \rangle_M$ on \mathbb{K}^n and a matrix $A \in \mathbb{K}^{n \times n}$ there exists a nonsingular matrix $X \in \mathbb{K}^{n \times n}$ such that $\tilde{A} = X^{-1}AX$ and $\tilde{M} = X^\#AX$ satisfy*

$$\tilde{A}^{\star_{\tilde{M}}} \tilde{A} = \begin{bmatrix} A_1 & 0 \\ 0 & A_0 \end{bmatrix}, \quad \tilde{M} = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix},$$

where the partitionings are conformal, A_1 is nonsingular, A_0 is nilpotent, and $X^\# = X^T$ in the case of a bilinear form or $X^\# = X^*$ in the case of a sesquilinear form. Moreover, if $A = WS$ where $W, S \in \mathbb{K}^{n \times n}$ and $\tilde{A} = X^{-1}WX \cdot X^{-1}SX \equiv \tilde{W}\tilde{S}$ then $\tilde{W}^{\star_{\tilde{M}}} = \tilde{W}^{-1}$ if and only if $\tilde{W}^{\star_{\tilde{M}}} = \tilde{W}^{-1}$ and S is M -selfadjoint if and only if \tilde{S} is \tilde{M} -selfadjoint.

The following result gives necessary and sufficient conditions for the existence of a generalized polar decomposition with a unique selfadjoint polar factor in the case of an orthosymmetric scalar product.

THEOREM 2.7 (generalized polar decomposition with unique selfadjoint factor). *Given an orthosymmetric scalar product $\langle \cdot, \cdot \rangle_M$ on \mathbb{K}^n , $A \in \mathbb{K}^{n \times n}$ has a generalized polar decomposition $A = WS$ with unique selfadjoint factor S if and only if*

- (a) $A^\star A$ has no negative real eigenvalues,
- (b) if zero is an eigenvalue of $A^\star A$ then it is semisimple, and
- (c) $\ker(A^\star A) = \ker(A)$.

Proof. By Lemma 2.6 we can assume without loss of generality that

$$(2.5) \quad A^\star A = B = \begin{bmatrix} B_1 & 0 \\ 0 & B_0 \end{bmatrix}, \quad M = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix},$$

where $B_1 \in \mathbb{K}^{k \times k}$ is nonsingular, $M_1 \in \mathbb{K}^{k \times k}$, and B_0 is nilpotent. Furthermore, we may assume that in the case of a sesquilinear form the matrix M is Hermitian. (If M satisfies $M^* = \alpha M$ for some $\alpha \in \mathbb{C}$ with $|\alpha| = 1$, let $\beta = \sqrt{\alpha}$ and replace M by the Hermitian matrix $\widetilde{M} = \beta M$. Note that a matrix is M -selfadjoint or an M -automorphism if and only if it is \widetilde{M} -selfadjoint or an \widetilde{M} -automorphism, respectively.)

(\Rightarrow) If $A = WS$ is a generalized polar decomposition then

$$A^*A = S^*W^*WS = S^2, \quad \ker(A) = \ker(S).$$

Since the nonzero eigenvalues of S lie in the open right half-plane, A^*A must have no negative real eigenvalues. In view of (2.5), since S commutes with A^*A it must have the form $S = \begin{bmatrix} S_1 & 0 \\ 0 & S_0 \end{bmatrix}$, where $S_1^2 = B_1$ and S_0 is nilpotent. Partition $W = \begin{bmatrix} W_1 & W_2 \\ W_3 & W_4 \end{bmatrix}$, where W_1 has the same size as S_1 and M_1 and set

$$(2.6) \quad \widetilde{W} = \begin{bmatrix} W_1 & -W_2 \\ W_3 & -W_4 \end{bmatrix}, \quad \widetilde{S} = \begin{bmatrix} S_1 & 0 \\ 0 & -S_0 \end{bmatrix}.$$

Then it is easily verified that $A = \widetilde{W}\widetilde{S}$ and that \widetilde{W} is an automorphism and \widetilde{S} is selfadjoint. As S_0 is nilpotent, S and \widetilde{S} have the same spectrum. Hence $A = \widetilde{W}\widetilde{S}$ is another generalized polar decomposition of A . Then the uniqueness of the selfadjoint polar factor implies $S = \widetilde{S}$ and thus $S_0 = 0$. Finally, we have $\ker(A^*A) = \ker(S) = \ker(A)$.

(\Leftarrow) From the semisimplicity of any eigenvalue zero of A^*A , we have $B_0 = 0$ in (2.5). From the condition $\ker(A^*A) = \ker(A)$ we obtain that A has the form $A = \begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix}$, where $A_1 \in \mathbb{K}^{k \times k}$. Since A^*A is M -selfadjoint it follows that B_1 is M_1 -selfadjoint. Let $S_1 = B_1^{1/2}$. Then

$$(2.7) \quad \begin{aligned} S_1^{*M_1} &= M_1^{-1}(B_1^{1/2})^*M_1 = M_1^{-1}(B_1^*)^{1/2}M_1 = (M_1^{-1}B_1^*M_1)^{1/2} \\ &= (B_1^{*M_1})^{1/2} = B_1^{1/2} = S_1, \end{aligned}$$

so S_1 is M_1 -selfadjoint. Next, define the $n \times n$ matrices

$$S = \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad W_0 = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix}.$$

Then S is M -selfadjoint, the nonzero eigenvalues of S lie in the open right half-plane, and $A^*A = S^2$. Moreover $A = W_0 S$ and

$$(2.8) \quad S^*W_0^*MW_0S = A^*MA = MA^*A = MS^2 = S^*MS,$$

i.e., W_0 preserves the scalar product on the subspace $\text{range } S$ of \mathbb{K}^n . Let $\widetilde{W}_0 : \text{range } S \rightarrow \text{range } A$ denote the restriction of the linear map $W_0 : \mathbb{K}^n \rightarrow \mathbb{K}^n$ to $\text{range } S$. Then \widetilde{W}_0 is bijective and because of (2.8) and by Witt's Theorem and the orthosymmetric property in Theorem 2.4, there exists an automorphism W such that $W|_{\text{range } S} = \widetilde{W}_0$. (Witt's Theorem is a classical result from algebra and can be found in many sources, such as [2, Thm. 2.1] and the references therein for the case of Hermitian sesquilinear or symmetric bilinear forms and, for the case of skew-symmetric bilinear forms, [2, Thm. 4.2] in the real case and [21, Thm. 1.1.18] in the case of an arbitrary field.) Clearly, W satisfies $A = WS$, so this is a generalized polar decomposition of A .

It remains to show that the selfadjoint polar factor is unique. To this end, let $A = \widetilde{W}\widetilde{S}$ be a second generalized polar decomposition. Then $A^*A = \widetilde{S}^2$ and $\ker(\widetilde{S}) = \ker(A) = \ker(A^*A)$, so \widetilde{S} has the form

$$\widetilde{S} = \begin{bmatrix} \widetilde{S}_1 & 0 \\ \widetilde{S}_2 & 0 \end{bmatrix},$$

where $\widetilde{S}_1 \in \mathbb{C}^{k \times k}$. Then

$$\begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix} = A^*A = \widetilde{S}^2 = \begin{bmatrix} \widetilde{S}_1^2 & 0 \\ \widetilde{S}_2\widetilde{S}_1 & 0 \end{bmatrix},$$

and the spectral requirements on \widetilde{S}_1 imply $\widetilde{S}_1 = B_1^{1/2} = S_1$, and then $\widetilde{S}_2 = 0$ since \widetilde{S}_1 is nonsingular. Hence $\widetilde{S} = S$, as required. \square

For the matrix A in (2.4) with nonunique generalized polar decomposition for M in (2.3), $A^*A = 0$, so conditions (a) and (b) of Theorem 2.7 are satisfied but condition (c) is not.

The proof of Theorem 2.7 shows that W is never unique when A is singular (since $\widetilde{W} \neq W$ in (2.6), as W is nonsingular). In the next section we develop a generalized polar decomposition in which both factors are unique under reasonable assumptions and which is defined for rectangular matrices of arbitrary shape.

3. The canonical generalized polar decomposition. We now consider rectangular matrices. Throughout this section we assume that \mathbb{K}^m and \mathbb{K}^n are equipped with scalar products induced by the nonsingular matrices $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$, respectively. For a matrix $A \in \mathbb{K}^{m \times n}$ the (M, N) -adjoint of A is defined to be the unique matrix $A^{*M, N} \in \mathbb{K}^{n \times m}$ satisfying the identity

$$\langle Ax, y \rangle_M = \langle x, A^{*M, N}y \rangle_N$$

for all $x \in \mathbb{K}^n$ and all $y \in \mathbb{K}^m$. Thus we have

$$A^{*M, N} = \begin{cases} N^{-1}A^T M, & \text{for bilinear forms,} \\ N^{-1}A^* M, & \text{for sesquilinear forms.} \end{cases}$$

Note that

$$(3.1a) \quad A \in \mathbb{K}^{m \times n}, B \in \mathbb{K}^{n \times m} \Rightarrow (AB)^{*M} = B^{*N, M} A^{*M, N},$$

$$(3.1b) \quad A \in \mathbb{K}^{m \times n}, B \in \mathbb{K}^{n \times n} \Rightarrow (AB)^{*M, N} = B^{*N} A^{*M, N},$$

$$(3.1c) \quad A \in \mathbb{K}^{m \times m}, B \in \mathbb{K}^{m \times n} \Rightarrow (AB)^{*M, N} = B^{*M, N} A^{*M}.$$

As a general rule, the adjoint of a product is the product in reverse order of the adjoints of the factors, where the relevant adjoint is determined by the dimensions of the factor.

DEFINITION 3.1. For a matrix $A \in \mathbb{K}^{m \times n}$ an (M, N) -Moore–Penrose pseudoinverse of A is a matrix $X \in \mathbb{K}^{n \times m}$ satisfying the conditions

$$(3.2) \quad \begin{array}{ll} \text{(i)} & AXA = A, \\ \text{(ii)} & XAX = X, \\ \text{(iii)} & AX = (AX)^{*M}, \\ \text{(iv)} & XA = (XA)^{*N}. \end{array}$$

The pseudoinverse is denoted by A^\dagger .¹

¹We do not find it necessary to include M and N in the notation.

In contrast to the usual Moore–Penrose pseudoinverse with $M = N = I$, an (M, N) -Moore–Penrose pseudoinverse need not always exist, as the following example shows for sesquilinear forms. Let

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad M = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad N \in \mathbb{K}^{2 \times 2} \text{ nonsingular}$$

and look for $X = A^\dagger$ of the form $X = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. Then (i) in (3.2) implies

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & c \\ 0 & 0 \end{bmatrix},$$

so that $c = 1$. On the other hand, (iii) gives

$$\begin{bmatrix} c & d \\ 0 & 0 \end{bmatrix} = AX = (AX)^{\star M} = \begin{bmatrix} 0 & \bar{d} \\ 0 & \bar{c} \end{bmatrix},$$

which implies $c = 0$, contradicting $c = 1$. Thus, A does not have an (M, N) -Moore–Penrose pseudoinverse.

However, if an (M, N) -Moore–Penrose pseudoinverse exists then it is unique. Indeed, let X, Y , be two (M, N) -Moore–Penrose pseudoinverses of A . Then, using (3.1a),

$$\begin{aligned} AX &= (AX)^{\star M} = X^{\star N, M} A^{\star M, N} = X^{\star N, M} A^{\star M, N} Y^{\star N, M} A^{\star M, N} \\ &= (AX)^{\star M} (AY)^{\star M} = AXAY = AY, \end{aligned}$$

and similarly $XA = YA$ can be shown. But then we have

$$X = XAX = XAY = YAY = Y.$$

For the rest of this section we need to restrict the scalar products. We need orthosymmetry of $\langle \cdot, \cdot \rangle_M$ and $\langle \cdot, \cdot \rangle_N$ together with an appropriate connection between them, which is formulated in the next definition.

DEFINITION 3.2. *The nonsingular matrices $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair if (a) for bilinear forms,*

$$M^T = \beta M, \quad N^T = \beta N, \quad \beta = \pm 1,$$

or (b) for sesquilinear forms,

$$(3.3) \quad M^* = \alpha M, \quad N^* = \alpha N, \quad \alpha \in \mathbb{C}, \quad |\alpha| = 1$$

(or, equivalently, $M = \beta G$, $N = \beta H$, where $\beta \in \mathbb{C}$, $|\beta| = 1$ and G and H are Hermitian).

Under the orthosymmetry assumption some useful relations hold for the adjoint.

LEMMA 3.3. *Let $A \in \mathbb{K}^{m \times n}$ and let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. Then*

- (a) $(A^{\star M, N} A)^{\star N} = A^{\star M, N} A$, that is, $A^{\star M, N} A$ is N -selfadjoint, and
- (b) $(A^{\star M, N})^{\star N, M} = A$.

Proof. For sesquilinear forms, we have, using (3.3),

$$\begin{aligned}(A^{\star_{M,N}}A)^{\star_N} &= N^{-1}(N^{-1}A^*MA)^*N = N^{-1}A^*M^*AN^{-*}N \\ &= N^{-1}A^*\alpha MA\alpha^{-1}N^{-1}N = N^{-1}A^*MA = A^{\star_{M,N}}A.\end{aligned}$$

Also, $(A^{\star_{M,N}})^{\star_{N,M}} = M^{-1}(N^{-1}A^*M)^*N = M^{-1}M^*AN^{-*}N = \alpha IA\alpha^{-1}I = A$. The proof for bilinear forms follows along the same lines. \square

We need the following generalization of partial isometry, which reduces to the usual partial isometry when $M = I$ and $N = I$.

DEFINITION 3.4. $W \in \mathbb{K}^{m \times n}$ is a partial (M, N) -isometry if $WW^{\star_{M,N}}W = W$.

The next result gives a useful characterization of partial (M, N) -isometry for an orthosymmetric pair.

THEOREM 3.5. Let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. $W \in \mathbb{K}^{m \times n}$ is a partial (M, N) -isometry if and only if $W^{\star_{M,N}} = W^\dagger$. If W is a partial (M, N) -isometry then

$$\langle Wx, Wy \rangle_M = \langle x, y \rangle_N \quad \text{for all } x, y \in \text{range}(W^{\star_{M,N}}).$$

Proof. The “if” follows immediately from $W = WW^\dagger W = WW^{\star_{M,N}}W$. For the “only if”, we have to show that $W^{\star_{M,N}}$ satisfies the conditions (3.2) of an (M, N) -Moore–Penrose pseudoinverse. The latter’s uniqueness then implies $W^{\star_{M,N}} = W^\dagger$. Indeed for sesquilinear forms, we have, using (3.3),

$$\begin{aligned}(WW^{\star_{M,N}})^{\star_M} &= M^{-1}(WN^{-1}W^*M)^*M = M^{-1}\alpha MW\alpha^{-1}N^{-1}W^*M \\ &= WN^{-1}W^*M = WW^{\star_{M,N}}, \\ (W^{\star_{M,N}}W)^{\star_N} &= N^{-1}(N^{-1}W^*MW)^*N = N^{-1}W^*\alpha MW\alpha^{-1}N^{-1}N \\ &= N^{-1}W^*MW = W^{\star_{M,N}}W,\end{aligned}$$

and thus, (iii) and (iv) are satisfied. Moreover, $WW^{\star_{M,N}}W = W$ (which is (i)) is satisfied by assumption and (ii) follows from

$$\begin{aligned}W^{\star_{M,N}}WW^{\star_{M,N}} &= N^{-1}W^*MWN^{-1}W^*M = N^{-1}W^*\alpha MW\alpha^{-1}N^{-1}W^*M \\ &= N^{-1}(WN^{-1}W^*MW)^*M = N^{-1}(WW^{\star_{M,N}}W)^*M \\ &= N^{-1}W^*M = W^{\star_{M,N}}.\end{aligned}$$

Finally, assume that W is a partial (M, N) -isometry and let $x, y \in \text{range}(W^{\star_{M,N}})$. Since $W^{\star_{M,N}} = N^{-1}W^*M$ and thus $\text{range}(W^{\star_{M,N}}) = \text{range}(N^{-1}W^*)$ this is equivalent to the existence of vectors z_x, z_y such that $x = N^{-1}W^*z_x$ and $y = N^{-1}W^*z_y$. Then we have

$$\begin{aligned}\langle Wx, Wy \rangle_M &= x^*W^*MWy = z_x^*W\alpha^{-1}N^{-1}W^*MWN^{-1}W^*z_y \\ &= \alpha^{-1}z_x^*WW^{\star_{M,N}}WN^{-1}W^*z_y = z_x^*W\alpha^{-1}N^{-1}W^*z_y \\ &= z_x^*WN^{-*}NN^{-1}W^*z_y = x^*Ny = \langle x, y \rangle_N.\end{aligned}$$

The case of bilinear forms is analogous. \square

For an example showing that the last part of Theorem 3.5 is not an if and only if statement, consider

$$W = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad M = N = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Then $W^{\star_{M,N}} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ and $\langle Wx, Wy \rangle_M = \langle x, y \rangle_N = 0$ for all $x, y \in \text{range}(W^{\star_{M,N}}) = \text{span}\{\begin{bmatrix} 0 \\ 1 \end{bmatrix}\}$. But, $W \neq WW^{\star_{M,N}}W = 0$ so W is not a partial (M, N) -isometry.

DEFINITION 3.6. *Let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. A canonical generalized polar decomposition of $A \in \mathbb{K}^{m \times n}$ is a decomposition $A = WS$, where $W \in \mathbb{K}^{m \times n}$ is a partial (M, N) -isometry, $S \in \mathbb{K}^{n \times n}$ is an N -selfadjoint matrix whose nonzero eigenvalues are contained in the open right half-plane, and $\text{range}(W^{\star_{M,N}}) = \text{range}(S)$.*

At this point, one may be tempted to define also a (non-canonical) generalized polar decomposition of $A \in \mathbb{K}^{m \times n}$, by analogy to the case for the standard Euclidean inner product, to be a decomposition $A = WS$, where $S \in \mathbb{K}^{n \times n}$ is N -selfadjoint and $W \in \mathbb{K}^{m \times n}$ satisfies $W^{\star_{M,N}}W = I_n$ if $m \geq n$ or $WW^{\star_{M,N}} = I_m$ if $m < n$. However, depending on M and N , such matrices W need not exist, irrespective of A . For example, let $\mathbb{K} = \mathbb{C}$ and

$$N = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad M = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Then there is no matrix W satisfying $I_2 = W^{\star_{M,N}}W = W^* \text{diag}(1, -1)W$, by Sylvester's law of inertia, so the intended decomposition does not exist for any A . The following lemma gives necessary conditions for the existence of canonical generalized polar decompositions.

LEMMA 3.7. *Let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. If $A \in \mathbb{K}^{m \times n}$ has the canonical generalized polar decomposition $A = WS$ then $A^{\star_{M,N}}A$ has no negative real eigenvalues, S is a square root of $A^{\star_{M,N}}A$, and*

$$(3.4) \quad W^{\star_{M,N}}WS = S.$$

Proof. By (3.1b), $A^{\star_{M,N}}A = S^{\star_N}W^{\star_{M,N}}WS = SW^{\star_{M,N}}WS$. Now for $z \in \mathbb{C}^n$, $Sz \in \text{range}(S) = \text{range}(W^{\star_{M,N}})$, so $Sz = W^{\star_{M,N}}u$ for some u . Then, since $W^{\star_{M,N}} = W^\dagger$ by Theorem 3.5,

$$(W^{\star_{M,N}}WS - S)z = W^{\star_{M,N}}WW^{\star_{M,N}}u - Sz = W^{\star_{M,N}}u - W^{\star_{M,N}}u = 0,$$

and since z is arbitrary (3.4) holds. Thus $A^{\star_{M,N}}A = SW^{\star_{M,N}}WS = S^2$. Since the nonzero eigenvalues of S lie in the open right half-plane this means that $A^{\star_{M,N}}A$ has no negative real eigenvalues. \square

The proof of our main theorem on the existence of a unique canonical generalized polar decomposition makes use of the following block diagonalization.

LEMMA 3.8. *Let $A \in \mathbb{K}^{m \times n}$ and let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. Then there exist nonsingular $X \in \mathbb{K}^{m \times m}$ and $Y \in \mathbb{K}^{n \times n}$ such that $\tilde{A} = X^{-1}AY$, $\tilde{M} = X^\#MX$, and $\tilde{N} = Y^\#NY$ satisfy*

$$\tilde{A}^{\star_{\tilde{M}, \tilde{N}}} \tilde{A} = \begin{bmatrix} A_1 & 0 \\ 0 & A_0 \end{bmatrix}, \quad \tilde{M} = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix}, \quad \tilde{N} = \begin{bmatrix} N_1 & 0 \\ 0 & N_0 \end{bmatrix},$$

where A_1 is nonsingular and A_0 is nilpotent, A_1 , M_1 , and N_1 have the same dimensions, and $\#$ denotes transpose for a bilinear form or conjugate transpose for a sesquilinear form. Moreover, if $A = WS$ where $W \in \mathbb{K}^{m \times n}$ and $S \in \mathbb{K}^{n \times n}$ and $\tilde{A} = X^{-1}WY \cdot Y^{-1}SY \equiv \tilde{W}\tilde{S}$ then W is a partial (M, N) -isometry if and only if \tilde{W} is a partial \tilde{M}, \tilde{N} -isometry and S is N -selfadjoint if and only if \tilde{S} is \tilde{N} -selfadjoint.

Proof. By Lemma 3.3, $A^{\star_{M,N}}A \in \mathbb{K}^{n \times n}$ is N -selfadjoint, so by Lemma 2.5 there exists a nonsingular $Y \in \mathbb{K}^{n \times n}$ such that

$$Y^{-1}A^{\star_{M,N}}AY = \begin{bmatrix} A_1 & 0 \\ 0 & A_0 \end{bmatrix}, \quad \tilde{N} = Y^{\#}NY = \begin{bmatrix} N_1 & 0 \\ 0 & N_0 \end{bmatrix},$$

where A_1 is nonsingular and A_0 is nilpotent.

For sesquilinear forms, since M is a normal matrix we can choose a nonsingular matrix $X \in \mathbb{K}^{m \times m}$ such that

$$(3.5) \quad \widetilde{M} = X^*MX = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix}$$

(indeed we can achieve a diagonal \widetilde{M}), with M_1 of the same dimensions as A_1 and N_1 . We have

$$\begin{aligned} \widetilde{A}^{\star_{\widetilde{M},\widetilde{N}}}\widetilde{A} &= \widetilde{N}^{-1}\widetilde{A}^*\widetilde{M}\widetilde{A} \\ &= Y^{-1}N^{-1}Y^{-*} \cdot Y^*A^*X^{-*} \cdot X^*MX \cdot X^{-1}AY \\ &= Y^{-1}N^{-1}A^*MAY = Y^{-1}A^{\star_{M,N}}AY = \begin{bmatrix} A_1 & 0 \\ 0 & A_0 \end{bmatrix}. \end{aligned}$$

The last part of the lemma is straightforward to verify.

Note that the decomposition (3.5) still holds with $*$ replaced by T for orthosymmetric bilinear forms on \mathbb{K}^n . Indeed by Definition 3.3, $M = \pm M^T$ and there exists an orthogonal matrix U when $\mathbb{K} = \mathbb{R}$ or unitary matrix U when $\mathbb{K} = \mathbb{C}$ such that $M = U\Sigma U^T$, where Σ is real and diagonal if $M = M^T$ (this is the symmetric SVD when $\mathbb{K} = \mathbb{R}$ and the Takagi factorization [13, Cor. 4.4.4] when $\mathbb{K} = \mathbb{C}$) or Σ is block diagonal with 2×2 blocks on the diagonal when $M = -M^T$ (the skew-symmetric Takagi factorization [13, Prob. 26, p. 217]). In the latter case the matrix N is skew-symmetric as well and it must be of even dimension since it is nonsingular; also, as $\widetilde{A}^{\star_{\widetilde{M},\widetilde{N}}}\widetilde{A}$ is \widetilde{N} -selfadjoint it has an even number of zero eigenvalues [18, Prop. 7.7] so that A_1 has even dimension. Hence for orthosymmetric bilinear forms there exists a nonsingular matrix X such that (3.5) holds with $*$ replaced by T . \square

THEOREM 3.9 (canonical generalized polar decomposition). *Let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. Then $A \in \mathbb{K}^{m \times n}$ has a unique canonical generalized polar decomposition if and only if*

- (a) $A^{\star_{M,N}}A$ has no negative real eigenvalues,
- (b) if zero is an eigenvalue of $A^{\star_{M,N}}A$ then it is semisimple, and
- (c) $\ker(A^{\star_{M,N}}A) = \ker(A)$.

Proof. By Lemma 3.8 we can assume that

$$(3.6) \quad A^{\star_{M,N}}A = \begin{bmatrix} B_1 & 0 \\ 0 & B_0 \end{bmatrix}, \quad M = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix}, \quad N = \begin{bmatrix} N_1 & 0 \\ 0 & N_0 \end{bmatrix},$$

where B_1 is nonsingular, $B_1, M_1, N_1 \in \mathbb{K}^{k \times k}$ for some $k \leq n$, and B_0 is nilpotent.

First, we consider the ‘‘if’’ part, so we assume that conditions (a)–(c) are satisfied. From (b) we have $B_0 = 0$ and (c) implies that A has the form

$$A = \begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix},$$

where $A_1 \in \mathbb{K}^{k \times k}$. For sesquilinear forms a simple computation yields

$$(3.7) \quad B_1 = N_1^{-1}(A_1^* M_1 A_1 + A_2^* M_0 A_2).$$

Lemma 3.3 shows that $A^{*M,N}A$ is N -selfadjoint, and it follows that B_1 is N_1 -selfadjoint. Let $S_1 = B_1^{1/2}$. Then S_1 is easily shown to be N_1 -selfadjoint (cf. (2.7)). Define

$$S = \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix} \in \mathbb{C}^{n \times n}, \quad W = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix} \in \mathbb{C}^{m \times n}.$$

Then S is N -selfadjoint with nonzero eigenvalues in the open right half-plane, $A = WS$, and

$$\begin{aligned} \text{range}(W^{*M,N}) &= \text{range}(N^{-1}W^*M) = \text{range}(N^{-1}W^*) \\ &= \text{range}\left(\begin{bmatrix} N_1^{-1}S_1^{-*}A_1^* & N_1^{-1}S_1^{-*}A_2^* \\ 0 & 0 \end{bmatrix}\right) \\ &= \left\{ \begin{bmatrix} x_1 \\ 0 \end{bmatrix} : x_1 \in \mathbb{C}^k \right\} = \text{range}\left(\begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix}\right) = \text{range}(S), \end{aligned}$$

since $[A_1^* \ A_2^*]$ has full rank, by virtue of $\ker(A^*A) = \ker(A)$. Moreover, W is a partial (M, N) -isometry, because using $N_1^{-1}S_1^{-*} = S_1^{-1}N_1^{-1}$, (3.7), and $B_1 = S_1^2$, we obtain

$$\begin{aligned} WW^{*M,N}W &= \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix} \begin{bmatrix} N_1^{-1}S_1^{-*}A_1^*M_1 & N_1^{-1}S_1^{-*}A_2^*M_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix} \\ &= \begin{bmatrix} A_1 S_1^{-1} N_1^{-1} S_1^{-*} A_1^* M_1 A_1 S_1^{-1} + A_1 S_1^{-1} N_1^{-1} S_1^{-*} A_2^* M_0 A_2 S_1^{-1} & 0 \\ A_2 S_1^{-1} N_1^{-1} S_1^{-*} A_1^* M_1 A_1 S_1^{-1} + A_2 S_1^{-1} N_1^{-1} S_1^{-*} A_2^* M_0 A_2 S_1^{-1} & 0 \end{bmatrix} \\ &= \begin{bmatrix} A_1 S_1^{-2} (N_1^{-1} A_1^* M_1 A_1 + N_1^{-1} A_2^* M_0 A_2) S_1^{-1} & 0 \\ A_2 S_1^{-2} (N_1^{-1} A_1^* M_1 A_1 + N_1^{-1} A_2^* M_0 A_2) S_1^{-1} & 0 \end{bmatrix} \\ &= \begin{bmatrix} A_1 S_1^{-2} B_1 S_1^{-1} & 0 \\ A_2 S_1^{-2} B_1 S_1^{-1} & 0 \end{bmatrix} = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix} = W. \end{aligned}$$

To prove uniqueness of the decomposition just established, let $A = \widetilde{W}\widetilde{S}$ be another decomposition, where \widetilde{W} is a partial (M, N) -isometry, \widetilde{S} is N -selfadjoint with nonzero spectrum in the open right half-plane, and $\text{range}(\widetilde{W}^{*M,N}) = \text{range}(\widetilde{S})$. First, we show that $\ker(A) = \ker(\widetilde{S})$. Clearly, the identity $A = \widetilde{W}\widetilde{S}$ implies $\ker(\widetilde{S}) \subseteq \ker(A)$. For the other inclusion, let $x \in \ker(A)$. Then, using (3.4), $0 = \widetilde{W}^{*M,N}Ax = \widetilde{W}^{*M,N}\widetilde{W}\widetilde{S}x = \widetilde{S}x$, so $x \in \ker(\widetilde{S})$, giving $\ker(A) \subseteq \ker(\widetilde{S})$. Therefore $\ker(A) = \ker(\widetilde{S})$. Hence \widetilde{S} has the form

$$\widetilde{S} = \begin{bmatrix} \widetilde{S}_1 & 0 \\ \widetilde{S}_2 & 0 \end{bmatrix},$$

where $\widetilde{S}_1 \in \mathbb{C}^{k \times k}$. Then, using Lemma 3.7,

$$\begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix} = A^{*M,N}A = \widetilde{S}^2 = \begin{bmatrix} \widetilde{S}_1^2 & 0 \\ \widetilde{S}_2 \widetilde{S}_1 & 0 \end{bmatrix},$$

and the spectral requirements on \widetilde{S}_1 imply that $\widetilde{S}_1 = B_1^{1/2} = S_1$, and then $\widetilde{S}_2 = 0$ since \widetilde{S}_1 is nonsingular. So $\widetilde{S} = S$. Let \widetilde{W} be partitioned conformably with \widetilde{S} , that

is,

$$\widetilde{W} = \begin{bmatrix} \widetilde{W}_1 & \widetilde{W}_2 \\ \widetilde{W}_3 & \widetilde{W}_4 \end{bmatrix}, \quad \text{or equivalently,} \quad \widetilde{W}^{\star_{M,N}} = \begin{bmatrix} N_1^{-1} \widetilde{W}_1^* M_1 & N_1^{-1} \widetilde{W}_3^* M_0 \\ N_0^{-1} \widetilde{W}_2^* M_1 & N_0^{-1} \widetilde{W}_4^* M_0 \end{bmatrix},$$

where $\widetilde{W}_1 \in \mathbb{C}^{k \times k}$. Then $\text{range}(\widetilde{W}^{\star_{M,N}}) = \text{range}(\widetilde{S})$ implies $\widetilde{W}_2 = 0$ and $\widetilde{W}_4 = 0$. Moreover, we obtain from the identity

$$\begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix} = A = \widetilde{W}S = \begin{bmatrix} \widetilde{W}_1 S_1 & 0 \\ \widetilde{W}_3 S_1 & 0 \end{bmatrix}$$

that $\widetilde{W}_1 = A_1 S_1^{-1}$ and $\widetilde{W}_3 = A_2 S_1^{-1}$, and hence $\widetilde{W} = W$, which concludes the proof of the uniqueness of the decomposition.

For the ‘‘only if’’ direction, suppose $A = WS$ is a unique canonical generalized polar decomposition. Since $S^2 = A^{\star_{M,N}}A$ by Lemma 3.7, S is a square root of $A^{\star_{M,N}}A$, commutes with $A^{\star_{M,N}}A$, and thus must have the form

$$S = \begin{bmatrix} S_1 & 0 \\ 0 & S_0 \end{bmatrix},$$

where $S_1^2 = B_1$ and S_0 is nilpotent. Since the nonzero eigenvalues of S_1 lie in the open right half-plane, $A^{\star_{M,N}}A$ must have no negative real eigenvalues. Partition $W = \begin{bmatrix} W_1 & W_2 \\ W_3 & W_4 \end{bmatrix}$, where $W_1 \in \mathbb{C}^{k \times k}$. Let

$$\widetilde{W} = \begin{bmatrix} W_1 & -W_2 \\ W_3 & -W_4 \end{bmatrix}, \quad \widetilde{S} = \begin{bmatrix} S_1 & 0 \\ 0 & -S_0 \end{bmatrix}.$$

Then it is easily verified that $A = \widetilde{W}\widetilde{S}$, \widetilde{W} is a partial (M, N) -isometry, \widetilde{S} is N -selfadjoint, and $\text{range}(\widetilde{S}) = \text{range}(\widetilde{W}^{\star})$. As S_0 is nilpotent, S and \widetilde{S} have the same spectrum. Hence $A = \widetilde{W}\widetilde{S}$ is another canonical generalized polar decomposition. Then the uniqueness of the decomposition implies $S = \widetilde{S}$ and thus $S_0 = 0$. From $A^{\star_{M,N}}A = S^2$ it then follows that if zero is an eigenvalue of $A^{\star_{M,N}}A$ then it is semisimple. Moreover, we have $\ker(A^{\star_{M,N}}A) = \ker(S) = \ker(A)$, where the latter equality follows from the argument given in the first part of the proof. \square

The next result shows that an analogue of the formula $A^+ = H^+U^+$ in Theorem 1.2 holds for the canonical generalized polar decomposition, provided that the decomposition is unique.

LEMMA 3.10. *Let $M \in \mathbb{K}^{m \times m}$ and $N \in \mathbb{K}^{n \times n}$ form an orthosymmetric pair. If $A \in \mathbb{C}^{m \times n}$ has the unique canonical generalized polar decomposition $A = WS$ then A and S have (M, N) -Moore-Penrose pseudoinverses A^\dagger and S^\dagger , respectively, which satisfy $A^\dagger = S^\dagger W^\dagger = S^\dagger W^{\star_{M,N}}$.*

Proof. By the proof of Theorem 3.9, we may assume that S and N have the forms

$$S = \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad N = \begin{bmatrix} N_1 & 0 \\ 0 & N_0 \end{bmatrix},$$

where $S_1, N_1 \in \mathbb{K}^{k \times k}$ and where S_1 is nonsingular. Then it is easy to check that

$$S^\dagger = \begin{bmatrix} S_1^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

is the (N, N) -Moore-Penrose pseudoinverse of S .

We now show that $X = S^\dagger W^{*M,N}$ satisfies the conditions (3.2). First, using (3.4), $AXA = WSS^\dagger W^{*M,N} WS = WSS^\dagger S = WS = A$. Next, using (3.4) again, $XAX = S^\dagger W^{*M,N} WSS^\dagger W^{*M,N} = S^\dagger S^\dagger W^{*M,N} = S^\dagger W^{*M,N} = X$. Then $XA = S^\dagger W^{*M,N} WS = S^\dagger S$ by (3.4), so by the definition of S^\dagger , $(XA)^{*N} = (S^\dagger S)^{*N} = S^\dagger S = XA$. Finally, $(AX)^{*M} = (WSS^\dagger W^{*M,N})^{*M} = (W^{*M,N})^{*N,M} (SS^\dagger)^{*N} W^{*M,N} = WSS^\dagger W^{*M,N} = AX$, by (3.1), Lemma 3.3 (b), and the definition of S^\dagger . \square

4. M -normal matrices. A matrix $A \in \mathbb{C}^{n \times n}$ is called M -normal with respect to a scalar product $\langle \cdot, \cdot \rangle_M$ if $A^*A = AA^*$. It is well known that in the case of the Euclidean scalar product a matrix is normal if and only if its polar factors commute [6]. For a scalar product $\langle \cdot, \cdot \rangle_M$ with Hermitian M , it is shown by Mehl, Ran, and Rodman [20, Thm. 10] that $A \in \mathbb{C}^{n \times n}$ allows a generalized polar decomposition $A = WS$ with commuting factors (here, no restrictions on the spectrum of S are imposed) if and only if A is M -normal and $\ker(A) = \ker(A^*)$. The following result shows that an analogous statement is true for our canonical generalized polar decomposition provided that the decomposition is unique.

THEOREM 4.1. *Let $A \in \mathbb{C}^{n \times n}$ have a unique canonical generalized polar decomposition $A = WS$ with respect to an orthosymmetric scalar product $\langle \cdot, \cdot \rangle_M$. Then the following statements are equivalent:*

- (a) A is M -normal,
- (b) $WS = SW$.

If (a) or (b) (and thus both) are satisfied then, in addition, $\ker(A) = \ker(A^*)$.

Proof. By Lemma 3.8 and the proof of Theorem 3.9 we may assume that

$$A = \begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix}, \quad S = \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad W = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix},$$

$$A^*A = \begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad M = \begin{bmatrix} M_1 & 0 \\ 0 & M_0 \end{bmatrix},$$

where B_1 is nonsingular, the partitionings are conformal, $[A_1^* \ A_2^*]$ has full rank, and $S_1 = B_1^{1/2}$. In particular, S_1 is a polynomial in B_1 [10, Thm. 1.29]. We now show the equivalence of the two statements.

(a) \Rightarrow (b): As A is M -normal, we have

$$\begin{bmatrix} B_1 & 0 \\ 0 & 0 \end{bmatrix} = A^*A = AA^* = \begin{bmatrix} A_1 M_1^{-1} A_1^* M_1 & A_1 M_1^{-1} A_2^* M_0 \\ A_2 M_1^{-1} A_1^* M_1 & A_2 M_1^{-1} A_2^* M_0 \end{bmatrix},$$

which implies $A_2 M_1^{-1} A_1^* = 0$ and $A_2 M_1^{-1} A_2^* = 0$, and thus $A_2 = 0$ as $[A_1^* \ A_2^*]$ has full rank. (In particular, this implies $\ker(A) = \ker(A^*)$.) In addition, we then have

$$M_1^{-1} A_1^* M_1 A_1 = (A^*A)_{11} = B_1 = A_1 M_1^{-1} A_1^* M_1.$$

Now A_1 commutes with B_1 , because

$$A_1 B_1 = A_1 M_1^{-1} A_1^* M_1 A_1 = B_1 A_1.$$

Thus, as S_1 is a polynomial in B_1 , A_1 also commutes with S_1 which implies

$$WS = \begin{bmatrix} A_1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} S_1 A_1 S_1^{-1} & 0 \\ 0 & 0 \end{bmatrix} = SW.$$

(b) \Rightarrow (a): Since W and S commute, we obtain that

$$(4.1) \quad \begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix} = WS = SW = \begin{bmatrix} S_1 A_1 S_1^{-1} & 0 \\ 0 & 0 \end{bmatrix},$$

which implies $A_2 = 0$ and thus $\ker A = \ker A^*$. (Since $[A_1^* \ A_2^*]$ has full rank, A_1 must be nonsingular if $A_2 = 0$.) It remains to show that A is M -normal or, equivalently, that A_1 is M_1 -normal. To this end, note that A_1 and S_1 commute by (4.1). Thus

$$M_1^{-1} A_1^* M_1 A_1 A_1 = B_1 A_1 = S_1^2 A_1 = A_1 S_1^2 = A_1 B_1 = A_1 M_1^{-1} A_1^* M_1 A_1,$$

that is, $M_1^{-1} A_1^* M_1 A_1 = A_1 M_1^{-1} A_1^* M_1$ because A_1 is nonsingular, or, equivalently, $A_1^{\star M_1} A_1 = A_1 A_1^{\star M_1}$, which means that A_1 is M_1 -normal. \square

5. Computational considerations. Much work has been done on computing the polar decomposition (see, for example, [4], [7], [15]) and more recently attention has been given to generalized polar decompositions [9], [12] and exploiting matrix automorphism group structure [11]. Here, we briefly consider computation of the canonical generalized polar decomposition. We begin with a key connection between iterations for the matrix sign function and iterations for the canonical generalized polar decomposition. Recall that for a matrix $A \in \mathbb{C}^{n \times n}$ with no pure imaginary eigenvalues the sign function can be defined by $\text{sign}(A) = A(A^2)^{-1/2}$ [8], [16]. The following theorem generalizes [12, Thm. 4.6]. See [8] or [10, Chap. 5] for details on the matrix sign function and its relation to the polar decomposition.

THEOREM 5.1. *Let $A \in \mathbb{K}^{m \times n}$ have a unique canonical generalized polar decomposition $A = WS$ and let M and N form an orthosymmetric pair. Let g be any scalar function of the form $g(x) = xh(x^2)$ such that*

- (a) *the iteration $X_{k+1} = g(X_k)$ converges to $\text{sign}(X_0)$ with order of convergence p whenever $\text{sign}(X_0)$ is defined,*
- (b) *$g(0) = 0$,*
- (c) *for sesquilinear forms, $g(X^{\star N}) = g(X)^{\star N}$ for all $X \in \mathbb{C}^{n \times n}$ in the domain of g .*

Then the iteration

$$(5.1) \quad Y_{k+1} = Y_k h(Y_k^{\star M, N} Y_k), \quad Y_0 = A$$

converges to W with order of convergence p .

Proof. By Lemma 3.8 and the proof of Theorem 3.9 we can assume that

$$A = \begin{bmatrix} A_1 & 0 \\ A_2 & 0 \end{bmatrix}, \quad S = \begin{bmatrix} S_1 & 0 \\ 0 & 0 \end{bmatrix}, \quad W = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_2 S_1^{-1} & 0 \end{bmatrix},$$

where the eigenvalues of S_1 lie in the open right half-plane. Let $X_{k+1} = g(X_k)$ with $X_0 = S$. By induction we easily obtain $X_k = \text{diag}(U_k, 0)$, where $U_{k+1} = g(U_k)$ and $U_0 = S_1$; the sequence $\{U_k\}$ is defined by assumption and condition (b) ensures that $g(X_k)$ is defined. Thus $X_k \rightarrow \text{diag}(\text{sign}(S_1), 0) = \text{diag}(I, 0)$ with order of convergence p by (a). Moreover, X_k is N -selfadjoint for all k by (c).

Next, we prove by induction that $Y_k = WX_k$. This is clearly true for $k = 0$. Assume it is true for k . Now X_k is a function of S , and hence a polynomial in S , and since $g(0) = 0$ the polynomial has zero constant term. It follows that $\text{range}(X_k) \subseteq \text{range}(S) = \text{range}(W^{\star M, N})$. Inspection of the proof of (3.4) shows that this identity

requires only $\text{range}(S) \subseteq \text{range}(W^{\star M, N})$. Hence $W^{\star M, N} W X_k = X_k$ and it follows, using (c), that

$$Y_{k+1} = W X_k h(X_k^{\star N} W^{\star M, N} W X_k) = W X_k h(X_k^{\star N} X_k) = W X_k h(X_k^2) = W X_{k+1}.$$

Thus $Y_{k+1} \rightarrow W \text{diag}(I, 0) = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_1 S_1^{-1} & 0 \end{bmatrix} \text{diag}(I, 0) = \begin{bmatrix} A_1 S_1^{-1} & 0 \\ A_1 S_1^{-1} & 0 \end{bmatrix} = W$. That the order of convergence is p is straightforward to show. (Note that the preservation of the p th order rate relies on the semisimplicity of the zero eigenvalue of $A^{\star M, N} A$. See [10, Sec. 6.3] for examples of iterations for the matrix square root that have quadratic convergence in general but only linear convergence for singular matrices.) \square

Assume for the rest of this section that M and N form an orthosymmetric pair and that $A \in \mathbb{C}^{m \times n}$ has a unique canonical generalized polar decomposition (or equivalently that the conditions in Theorem 3.9 hold).

Theorem 5.1 shows that we can convert iterations for the matrix sign function into iterations for the canonical generalized polar decomposition. The required form of the iteration function g is not restrictive; indeed, all iterations in the Padé family have g of the form in the theorem [10, Sec. 5.4]. Consider the [0/1] Padé iteration

$$(5.2) \quad S_{k+1} = 2S_k(I + S_k^2)^{-1}, \quad S_0 = S \in \mathbb{C}^{n \times n},$$

for which $S_k \rightarrow \text{sign}(S)$ quadratically. Theorem 5.1 yields the iteration

$$(5.3) \quad X_{k+1} = 2X_k \left(I + X_k^{\star M, N} X_k \right)^{-1}, \quad X_0 = A \in \mathbb{C}^{m \times n}$$

and shows that $X_k \rightarrow W$ quadratically, where $A = WS$ is the canonical generalized polar decomposition.

Having computed W , how can we obtain S ? From (3.4) we have the formula

$$(5.4) \quad S = W^{\star M, N} W S = W^{\star M, N} A.$$

We give two numerical examples. First,

$$A = \begin{bmatrix} \alpha & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & \beta \end{bmatrix}, \quad M = N = \begin{bmatrix} 0 & -I_2 \\ I_2 & 0 \end{bmatrix}.$$

We examine three cases.

(a) $\alpha = 2, \beta = 0$: $A^{\star M, N} A$ has only zero eigenvalues, occurring in two Jordan blocks of size 2, and $\dim(\ker(A)) = 1 < 2 = \dim(\ker(A^{\star M, N} A))$, so conditions (b) and (c) in Theorem 3.9 are violated. Iteration (5.3) does not converge. In fact, A does not have a canonical generalized polar decomposition. Indeed, if $A = WS$ were to be such a decomposition then S would satisfy $\ker(A) = \ker(S)$. Now a straightforward calculation shows that any matrix satisfying $S^T M = M S$ and $\ker(S) = \ker(A)$ must be of the form

$$S = \begin{bmatrix} s_{11} & 0 & 0 & s_{14} \\ s_{21} & -s_{14} & -s_{14} & 0 \\ 0 & s_{11} & s_{11} & s_{21} \\ -s_{11} & 0 & 0 & -s_{14} \end{bmatrix}.$$

Such matrices S , however, have rank at most two while A has rank three, so there does not exist any M -selfadjoint matrix with $\ker(A) = \ker(S)$.

(b) $\alpha = 3, \beta = 2$: $A^{\star_{M,N}}A$ has spectrum $\{3, 3, 0, 0\}$ with semisimple zero eigenvalue, and $\dim(\ker(A)) = 1 < 2 = \dim(\ker(A^{\star_{M,N}}A))$. Condition (c) in Theorem 3.9 is violated and iteration (5.1) does not converge. The same argument as in the previous case shows that A does not have a canonical generalized polar decomposition.

(c) $\alpha = 3, \beta = 1$: $A^{\star_{M,N}}A$ has spectrum $\{2, 2, 0, 0\}$ with semisimple zero eigenvalue, and $\dim(\ker(A)) = 2 = \dim(\ker(A^{\star_{M,N}}A))$, so Theorem 3.9 ensures the existence of a unique canonical generalized polar decomposition $A = WS$, where the factors can be shown to be

$$W = \frac{1}{\sqrt{2}} \begin{bmatrix} 3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad S = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & 0 & 0 & 0 \end{bmatrix}.$$

Iteration (5.3) produces iterates with relative differences $\|X_k - X_{k-1}\|_1 / \|X_k\|_1$ equal to 5.00e-1, 5.56e-2, 1.73e-3, 1.50e-6, 1.13e-12, 1.05e-16, at which point it has converged to the working precision in the MATLAB environment used, for which the unit roundoff $u = 2^{-53} \approx 1.1 \times 10^{-16}$. The expected quadratic convergence is evident. The conditions (3.2) are all found to be satisfied to working precision by the computed W , thus verifying that $W^{\star_{M,N}}$ is a partial (M, N) -isometry (see Theorem 3.5), the computed S is N -selfadjoint to working precision, and the relative residual $\|A - WS\|_1 / \|A\|_1$ is also of order the working precision.

For the second example,

$$A = \begin{bmatrix} 1 & 2 & 2 & 2 & 2 & 2 \\ 0 & 1 & 2 & 2 & 2 & 2 \\ 0 & 0 & 1 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 & 2 & 2 \end{bmatrix}, \quad M = \begin{bmatrix} 0 & -I_2 \\ I_2 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & -I_3 \\ I_3 & 0 \end{bmatrix}.$$

Here, $A^{\star_{M,N}}A$ has diagonal Jordan form with two zero eigenvalues and conditions (a)–(c) in Theorem 3.9 are all satisfied. Indeed, A has a unique canonical generalized polar decomposition $A = WS$, where $W = W_1/(6\sqrt{2})$ and $S = S_1/(6\sqrt{2})$, with

$$W_1 = \begin{bmatrix} 8 & 7 & -2 & 2 & 6 & 6 \\ -4 & 2 & 8 & 4 & 4 & 4 \\ 0 & -2 & 4 & 8 & 4 & 4 \\ 2 & 4 & -5 & -4 & 6 & 6 \end{bmatrix}, \quad S_1 = \begin{bmatrix} 8 & 12 & 6 & 0 & -4 & -4 \\ 4 & 14 & 14 & 4 & 0 & 0 \\ 4 & 14 & 14 & 4 & 0 & 0 \\ 0 & -2 & 4 & 8 & 4 & 4 \\ 2 & 0 & 3 & 12 & 14 & 14 \\ -4 & -3 & 0 & 6 & 14 & 14 \end{bmatrix}.$$

Iteration (5.3) produces iterates with relative differences $\|X_k - X_{k-1}\|_1 / \|X_k\|_1$ equal to 3.03e-1, 1.61e-1, 2.10e-2, 2.55e-4, 3.62e-8, and 9.89e-16. Again, quadratic convergence is evident and the computed W and S satisfy the expected equations to working precision.

6. Conclusions. We have introduced the canonical generalized polar decomposition $A = WS$ for rectangular matrices $A \in \mathbb{K}^{m \times n}$ of arbitrary dimensions with respect to scalar products in \mathbb{K}^m and \mathbb{K}^n induced by nonsingular matrices M and N . Under the assumption of orthosymmetry of the scalar products we have obtained necessary and sufficient conditions for the existence of a unique canonical generalized polar decomposition and have shown that (a) various relations and identities for the standard polar decomposition hold in appropriately generalized forms and (b) the

(M, N) -Moore–Penrose pseudoinverse and the partial (M, N) -isometry play a fundamental role. Since the canonical generalized polar decomposition can, moreover, be computed by adapting iterations for the matrix sign function this decomposition is arguably the “right” generalization of the polar decomposition to indefinite inner product spaces from a computational standpoint.

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