H-selfadjoint roots of H-selfadjoint matrices and H-polar decompositions over the quaternions

M van Straaten

orcid.org/0000-0001-5345-2842

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Promoter:	Prof ACM Ran
Co-promoter:	Dr F Theron
Co-promoter:	Dr DB Janse van Rensburg
Assistant Promoter:	Prof GJ Groenewald

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Abstract

All vector spaces in this thesis will be endowed with an indefinite inner product defined by an invertible Hermitian matrix H. We study cases where the H has either complex or quaternion entries depending on the context.

We generalize known results on the existence of an H-selfadjoint square root of an H-selfadjoint complex matrix to the existence of an H-selfadjoint mth root. It is found that the conditions on an H-selfadjoint complex matrix B ensuring the existence of an H-selfadjoint mth root, are only necessary for the blocks with eigenvalue zero and the blocks with negative eigenvalues. The results are given as conditions on the canonical form of (B, H) and although the results associated with the negative eigenvalues are the same as in the square root case, the results associated with the zero eigenvalue are somewhat more intricate. A construction for an H-selfadjoint mth root is included in each of the proofs for different cases depending on the eigenvalues.

The study of square roots of H-nonnegative complex matrices is interesting because of the simple structure of these matrices. For each of the three cases, namely for square roots, H-selfadjoint square roots and H-nonnegative square roots of H-nonnegative matrices, we give necessary and sufficient conditions for the existence of a square root and we describe the square roots for the blocks with zero eigenvalue. The Jordan normal form is obtained for a square root of an H-nonnegative matrix and for the cases where A is an H-selfadjoint square root or an H-nonnegative square root of an H-nonnegative matrix, a canonical form of (A, H) is obtained. Conditions are also found for an H-nonnegative square root to be stable.

We extend the complex case of H-selfadjoint mth roots to the skew field of quaternions and using the complex matrix representation of quaternion matrices, we prove that the results are essentially the same in the quaternion case as in the complex case, despite the noncommutativity of quaternions.

Due to a logical connection between square roots and polar decompositions, it is natural to study H-polar decompositions of quaternion matrices. We show that a quaternion matrix X admits an H-polar decomposition, say $X = UA$ for an H-selfadjoint matrix A and an H-unitary matrix U, if and only if the matrix $X^{[*]}X$ has an H-selfadjoint square root A and the null spaces of X and A coincide. Specialising the conditions we found for the existence of an H-selfadjoint mth root to the case $m = 2$, we conclude by giving the conditions in terms of the canonical form of the pair $(X^{[*]}X, H)$ and a basis for the null space of X. We also prove that Witt's theorem is true for quaternion matrices.

Keywords: H-selfadjoint matrix, mth root, H-polar decomposition, Quaternion, H-nonnegative matrix, Indefinite inner product.

Summary

Throughout this thesis we work with an indefinite inner product which is defined on either a complex vector space or a quaternion vector space. A function $[\cdot,\cdot]$ from $\mathbb{C}^n \times \mathbb{C}^n$ to $\mathbb{C}$ is called an indefinite inner product in $\mathbb{C}^n$ if it is linear in the first argument, anti-symmetric and nondegenerate. Every indefinite inner product is defined by an invertible Hermitian matrix $H \in \mathbb{C}^{n\times n}$ as follows: $[x, y] = \langle Hx, y\rangle$ for $x, y \in \mathbb{C}^n$ (where $\langle\cdot,\cdot\rangle$ denotes the standard inner product). One could also substitute the set of quaternions $\mathbb{H}$ for $\mathbb{C}$.

A square matrix A is called an mth root of a square matrix B if $A^m = B$, where m is any positive integer. The matrix $\bar{A}$ is the matrix in which each entry is the conjugate of the corresponding entry in A and the transpose of the matrix $\bar{A}$ is denoted by A^*. Let $J_n(\lambda)$ denote a single $n \times n$ Jordan block with eigenvalue $\lambda \in \mathbb{C}$ and let Q_n denote the $n \times n$ matrix with ones on the main anti-diagonal and zeros elsewhere, called the sip (standard involutory permutation) matrix. The usual notation $\sigma(A)$ is used for the set of eigenvalues of a matrix A. The H-adjoint of a matrix $A \in \mathbb{C}^{n\times n}$ is the unique $n \times n$ matrix $A^{[*]}$ such that $[Ax, y] = [x, A^{[*]}y]$ for all $x, y \in \mathbb{C}^n$. A matrix A is said to be H-selfadjoint if $A = A^{[*]}$, or equivalently if $HA = A^*H$, and A is called H-unitary if A is invertible and $A^{-1} = A^{[*]}$, or equivalently if $A^*HA = H$. In the case where we have two indefinite inner products $[\cdot,\cdot]_1$ and $[\cdot,\cdot]_2$ on $\mathbb{C}^n$ which are defined by invertible Hermitian matrices $H_1, H_2 \in \mathbb{C}^{n\times n}$, and a linear transformation $U : \mathbb{C}^n \to \mathbb{C}^n$ satisfying $[Ux, Uy]_2 = [x, y]_1$ for every $x, y \in \mathbb{C}^n$, the transformation U is said to be H_1-H_2-unitary.

There exists a unique canonical form $(S^{-1}AS, S^*HS)$ (up to permutation of corresponding blocks) for each pair (A, H) where A is H-selfadjoint and S is invertible. The matrix $S^{-1}AS$ consists of a direct sum of Jordan blocks and S^*HS consists of a direct sum of sip matrices. For a real λ_i, the Jordan block $J_{k_i}(\lambda_i)$ corresponds to a matrix $\varepsilon_i Q_{k_i}$ in the canonical form. It is said that the block $J_{k_i}(\lambda_i)$ has positive sign characteristic if $\varepsilon_i = 1$ and negative sign characteristic if $\varepsilon_i = -1$. Let $A \in \mathbb{C}^{n\times n}$ be a matrix which has $\bigoplus_{i=1}^{r} J_{n_i}(\lambda)$ at the eigenvalue λ in its Jordan normal form and assume that the sizes are in decreasing order. Then the Segre characteristic of A corresponding to the eigenvalue λ is defined as the sequence $n_1, n_2, n_3, \ldots, n_r, 0, 0, \ldots$.

A matrix $A \in \mathbb{C}^{n\times n}$ is called H-nonnegative if $[Ax, x] \geq 0$ for all $x \in \mathbb{C}^n$. It is known that an H-nonnegative matrix is H-selfadjoint, has only real eigenvalues and all of its Jordan blocks are of size one except Jordan blocks with eigenvalue zero which are of size at most two. Moreover, the Jordan blocks with positive (respectively, negative) eigenvalues have positive (respectively, negative) sign characteristic and the blocks $J_2(0)$ have positive sign characteristic. In this setting, we also define a Segre pairing. Let $n_1, n_2, \ldots, n_r$ be the Segre characteristic of a nilpotent H-nonnegative matrix A. Note that the zeros are dropped here but they are considered in the definition. We call a collection $\mathcal{S}$ of pairs of numbers from $\mathcal{N} = \{n_i\}_{i=1}^{r} \cup \{0\}$ a Segre pairing if:

- each entry in the Segre characteristic appears in one and only one pair of $\mathcal{S}$;
- each pair in $\mathcal{S}$ consists of two entries from the Segre characteristic or one entry from the Segre characteristic and one zero, with the first entry greater or equal to the second entry;
- the absolute difference between the two entries in each pair is at most one;
- the pairs are arranged lexicographically.

Firstly, we want to generalize known results on the existence of an H-selfadjoint square root of an H-selfadjoint complex matrix to the existence of an H-selfadjoint mth root. For an H-selfadjoint matrix B, we find that there exists an H-selfadjoint mth root if and only if the canonical form of (B, H) has the following three properties: in the case where m is even, the Jordan blocks of B with negative eigenvalues α_j can be reordered as a direct sum of pairs $J_{k_j}(\alpha_j) \oplus J_{k_j}(\alpha_j)$ and the two blocks in each pair have opposite sign characteristic. The other two properties regarding the zero eigenvalue of B are as follows: there exists a reordering of the Segre characteristic of B corresponding to the zero eigenvalue such that the difference between any two entries in each m-tuple is at most one, and specific rules hold for the number of Jordan blocks with positive sign characteristic. The proof is split into several cases depending on the eigenvalues, in particular, for the cases where B has only positive eigenvalues, only nonreal eigenvalues, only eigenvalue zero, and only negative eigenvalues (two separate cases here for m even and for m odd). Included in the proofs are constructions for H-selfadjoint mth roots when they exist. The relation between the canonical forms of (A, H) and (A^m, H) for the case where A has only the eigenvalue zero, is also found.

Secondly, square roots of H-nonnegative complex matrices are studied because the simple structure makes explicit description of the roots possible. We show that an H-nonnegative matrix B has a square root if and only if in the Segre characteristic of B corresponding to the eigenvalue zero there is either an even number of entries equal to two, or there is an odd number of entries equal to two and at least one entry equal to one. In the second part, it is shown that B has an H-selfadjoint square root if and only if B has no negative eigenvalues and the number of Jordan blocks $J_1(0)$ with positive sign characteristic is not less than the number of Jordan blocks $J_2(0)$. This is a result of only being able to pair ones with twos, in the Segre pairing, and not twos with twos. When we restrict the square root of B further to be H-nonnegative, the conditions are found to be as follows: B has no negative eigenvalues and no Jordan blocks of size two with eigenvalue zero.

We also obtain the explicit forms of the square roots, H-selfadjoint square roots and H-nonnegative square roots of a nilpotent H-nonnegative matrix in Jordan normal form. From these results the Jordan normal form is deduced for a square root of an H-nonnegative matrix and for the cases where A is an H-selfadjoint square root or an H-nonnegative square root of an H-nonnegative matrix, a canonical form of (A, H) is

obtained. In the final section of this part of the research we study the notion of stability. An H-nonnegative square root A of an H-nonnegative matrix B is called unconditionally stable if for all $\varepsilon > 0$ there exists a $\delta > 0$ such that for all H-nonnegative matrices $\tilde{B}$ satisfying $\|B - \tilde{B}\| < \delta$, $\tilde{B}$ has an H-nonnegative square root $\tilde{A}$ for which $\|A - \tilde{A}\| < \varepsilon$. We prove that an H-nonnegative matrix B has an unconditionally stable H-nonnegative square root A if and only if there is no pair $(1, 1)$ in the Segre pairing of B and all Jordan blocks $J_1(0)$ associated with the pair $(1, 0)$ have positive sign characteristic. Restricting ourselves to only the H-nonnegative matrices $\tilde{B}$ having at least one H-nonnegative square root, we show that B has a conditionally stable H-nonnegative square root A if and only if there is no pair $(1, 1)$ in the Segre pairing of B.

Thirdly, we extend our study of H-selfadjoint mth roots to the skew field of quaternions. The complex matrix representation of quaternion matrices is used to simplify the problem. If A is an $n \times n$ quaternion matrix written as $A = A_1 + \mathrm{j}A_2$ where $A_1, A_2 \in \mathbb{C}^{n\times n}$, then the map $\omega_n : \mathbb{H}^{n\times n} \to \mathbb{C}^{2n\times 2n}$ defined by

$$\omega_n(A) = \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix}$$

is an isomorphism of $\mathbb{H}^{n\times n}$ onto the real unital subalgebra Ω_{2n} of $\mathbb{C}^{2n\times 2n}$, where

$$\Omega_{2n} := \left\{ \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix} \mid A_1, A_2 \in \mathbb{C}^{n\times n} \right\}.$$

Using the canonical form of a pair of quaternion matrices and the properties of ω_n, we present the canonical form of a pair of matrices in Ω_{2n}. The main result in this part of the research is necessary and sufficient conditions for the existence of an H-selfadjoint mth root of an H-selfadjoint matrix where all matrices are in Ω_{2n}. It is important to first show that there exists an H-selfadjoint matrix A such that $A^m = B$ if and only if there exists an $\omega_n(H)$-selfadjoint matrix $\omega_n(A)$ such that $(\omega_n(A))^m = \omega_n(B)$, where $\omega_n(B)$ is an $\omega_n(H)$-selfadjoint matrix in the subalgebra Ω_{2n}.

We prove that $B \in \Omega_{2n}$ has an H-selfadjoint mth root in Ω_{2n} if and only if the part of the canonical form of (B, H) with negative eigenvalues is equal to (B_-, H_-) when m is even and the part of the canonical form with eigenvalue zero is equal to (B_0, H_0), where these matrices are as follows:

$$B_- = \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \right) \oplus \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \right),$$

$$H_- = \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j} \right) \oplus \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j} \right),$$

where $\lambda_j < 0$; and

$$B_0 = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=r_j+1}^{m} J_{a_j}(0) \right) \oplus \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=r_j+1}^{m} J_{a_j}(0) \right),$$

$$H_0 = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right) \oplus \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right),$$

for some $a_j, r_j \in \mathbb{Z}$ with $0 < r_j \leq m$. The signs are as follows, given in terms of η_j, where η_j could be either 1 or -1: If r_j (respectively $m - r_j$) is even, half of $\varepsilon_i^{(j)}$ for $i = 1, \ldots, r_j$ (respectively for $i = r_j + 1, \ldots, m$) are equal to η_j and the other half are equal to $-\eta_j$. If r_j (respectively $m - r_j$) is odd, there is one more of the $\varepsilon_i^{(j)}$ for $i = 1, \ldots, r_j$ (respectively for $i = r_j + 1, \ldots, m$) equal to η_j than to $-\eta_j$.

Consequently, by applying the inverse of ω_n, the conditions are found to be essentially the same in the quaternion case as in the complex case, despite the noncommutativity of quaternions.

For the last part of this thesis, the objective is to find necessary and sufficient conditions for a quaternion matrix X to admit an H-polar decomposition. We extend Witt's theorem to the quaternion case, that is, we prove that if there is a nonsingular linear transformation U_0 between subspaces V_1 and V_2 in $\mathbb{H}^n$ satisfying $[U_0x, U_0y]_2 = [x, y]_1$ for every $x, y \in V_1$ where the two defining matrices H_1 and H_2 have the same number of positive eigenvalues, then there exists an H_1-H_2-unitary linear transformation U which satisfies $Ux = U_0x$ for every $x \in V_1$. This U is called a Witt extension of U_0. In a subsequent result we also present the form of any Witt extension.

The main result in this part is that $X \in \mathbb{H}^{n \times n}$ admits an H-polar decomposition, that is, $X = UA$ where A is an H-selfadjoint matrix and U is an H-unitary matrix, if and only if the matrix $X^{[*]}X$ has an H-selfadjoint square root A such that the null spaces of X and A coincide. This is shown by obtaining an injective H_2-isometry U_0 satisfying $X = U_0A$ and then using Witt's theorem to extend U_0 to an H-unitary matrix U. Finally, the conditions for the existence of an H-polar decomposition for X are given in terms of the canonical form of the pair $(X^{[*]}X, H)$ with the help of the conditions found for H-selfadjoint mth roots (here only for the case $m = 2$), as well as a basis for the null space of X.

Preface

For this thesis the article format has been selected. The research was structured for this format from the outset, and four papers were produced, all of which were accepted at accredited journals.

The co-authors of the papers mostly took the role of advisers in the research process, whereas the student focused on developing proofs as well as formulation of results. Hence the student had an absolute majority share by far.

Up to some minor modifications, the chapters included in this thesis were published as papers in two academic journals. In the same order as the chapters, the publications are as follows:

1. G.J. Groenewald, D.B. Janse van Rensburg, A.C.M. Ran, F. Theron, M. van Straaten. mth roots of H-selfadjoint matrices, *Linear Algebra and its Applications*, **610**, (2021), 804–826.

2. D.B. Janse van Rensburg, M. van Straaten, F. Theron, C. Trunk. Square roots of H-nonnegative matrices, *Linear Algebra and its Applications*, **621**, (2021), 29–49.

3. D.B. Janse van Rensburg, A.C.M. Ran, F. Theron, M. van Straaten. mth roots of H-selfadjoint matrices over the quaternions, *Electronic Journal of Linear Algebra*, **37**, (2021), 492–503.

4. G.J. Groenewald, D.B. Janse van Rensburg, A.C.M. Ran, F. Theron, M. van Straaten. Polar decompositions of quaternion matrices in indefinite inner product spaces, *Electronic Journal of Linear Algebra*, **37**, (2021), 659–670.

All of the listed co-authors gave permission that the research in the published papers may be presented as part of the thesis and to be submitted in fulfilment of the requirements of the student's doctoral degree.

Contents

Chapter 1

Introduction

The central topic of this thesis is the study of mth roots of both complex and quaternion matrices, where m is any positive integer. Extra conditions are imposed on the matrices and/or their roots while working with an indefinite inner product. Ultimately, we apply the results on roots in the study of polar decompositions. Let us start by introducing a few necessary notions.

A square matrix A is called an mth root of a square matrix B if $A^m = B$. Throughout this thesis we work with an indefinite inner product which is defined on either the complex vector space or the quaternion vector space. In the following definitions one could also substitute the set of quaternions $\mathbb{H}$ for $\mathbb{C}$. Every indefinite inner product is defined by an invertible Hermitian matrix $H \in \mathbb{C}^{n\times n}$ as follows: $[x, y] = \langle Hx, y\rangle$ for $x, y \in \mathbb{C}^n$ (where $\langle \cdot\,, \cdot\rangle$ denotes the standard inner product). A matrix $A \in \mathbb{C}^{n\times n}$ is called *H-selfadjoint* if it is selfadjoint with respect to the indefinite inner product determined by H, or equivalently if $HA = A^*H$, and A is called *H-unitary* if A is invertible and $A^*HA = H$. Lastly, A is called *H-nonnegative* if $[Ax, x] \geq 0$ for all $x \in \mathbb{C}^n$. The $n \times n$ matrix in which each entry is the conjugate of the corresponding entry in A is denoted by $\bar{A}$ and the transpose of $\bar{A}$ is the $n \times n$ matrix denoted by A^*.

For background on indefinite inner product spaces in finite dimensional spaces, a great start is the book by Gohberg, Lancaster and Rodman [14]. The book by Leiba Rodman [22] contains an extensive narrative on quaternion linear algebra.

The main research questions that are answered in the thesis may be stated as follows: Find necessary and sufficient conditions for the existence of an H-selfadjoint mth root, say A, of a square H-selfadjoint complex matrix B, that is, $A^m = B$. In particular, develop a construction for such an H-selfadjoint mth root.

Next, for an H-nonnegative matrix obtain necessary and sufficient conditions for the existence of a square root under no restrictions, of an H-selfadjoint square root and also of an H-nonnegative square root. Characterize all square roots, all H-selfadjoint square roots and all H-nonnegative square roots of H-nonnegative complex matrices. Furthermore, study the existence of a stable H-nonnegative square root of an H-nonnegative matrix. The reason for the study of roots of H-nonnegative matrices is that this class is a significant subclass of the class of H-selfadjoint matrices, and it has a simple structure which is easily described explicitly.

A similar question to the first research question above can be asked in the quaternion case, that is, find necessary and sufficient conditions for the existence of an H-selfadjoint mth root of an H-selfadjoint quaternion matrix. For this part, the complex matrix representation of a quaternion matrix is used to simplify the proofs.

Finally, find necessary and sufficient conditions on a given square quaternion matrix X for the existence of an H-polar decomposition of X in terms of an H-unitary matrix U and an H-selfadjoint matrix A, such that $X = UA$. This is a natural sequel to the study of square roots in an indefinite inner product space, since the study of polar decompositions is closely related to that of square roots.

In the following sections we present some background material and discuss the development of the theory in existing literature. The last section of this introduction, in the form of a structure overview, gives an idea of what can be expected throughout the thesis by introducing some of the results in a way which is perhaps easier to digest. Note that we use standard terminology from linear algebra which can be found in many books, see for example the book by Horn and Johnson [16].

1.1 Roots of matrices

Roots of matrices have been studied extensively, from as early as 1858 in the paper by Cayley [9]. For a short account of the further development of the roots of matrices, see Section 5 of Drazin [12]. Cross and Lancaster [10] found in 1974 necessary and sufficient conditions for the existence of square roots of complex matrices by using dimensions of null spaces of powers of the matrix. Let m be any positive integer. In [21] Psarrakos obtained a criterion for the existence of mth roots of singular matrices by using elementary divisors. A Schur algorithm is used in the paper by Smith [24] to find mth roots in the nonsingular case, building on results of Björk and Hammarling [3] and of Higham [15]. On the other hand, in the paper by Borwein and Richmond [8], conditions are given for the existence of mth roots of nilpotent matrices in terms of the sizes of the Jordan blocks. This was especially useful in our research. For easy reference we also state the result here:

Theorem 1.1.1 (Theorem 2, [8]). *The $n \times n$ complex matrix B has an mth root A, that is, $A^m = B$, if and only if the dimensions n_i of the blocks in the Jordan normal form of B with eigenvalue zero, in decreasing order, satisfy*

$$n_{rm+1} - n_{(r+1)m} \leq 1, \quad 0 \leq r \leq s-1,$$

where $\sum_{i=1}^{sm} n_i$ is the total dimension of the blocks in the Jordan normal form of B with eigenvalue zero and we assume there are exactly sm such blocks.

Let $J_k(\lambda)$ denote the single $k \times k$ Jordan block with the eigenvalue λ. The Jordan normal form of a matrix B is the matrix J consisting of a direct sum of Jordan blocks where J is similar to B and unique up to a permutation of diagonal blocks. Theorem 1.1.1 is true because of the fact that the matrix $(J_{am+r}(0))^m$ is similar to the direct sum

$$\bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0)$$

as is illustrated by the following example.

Example 1.1.2. Consider the two Jordan blocks with eigenvalue zero and sizes $n = 7$ and $n = 8$. Raise both of these matrices to the mth power and then find the Jordan normal form. If $m = 2$, then both $(J_7(0))^2$ and $(J_8(0))^2$ are matrices with ones on the second superdiagonal and zeros elsewhere. From the Jordan normal form of these two matrices we then obtain:

$$\begin{aligned} (J_7(0))^2 &\text{ is similar to } J_4(0) \oplus J_3(0); \\ (J_8(0))^2 &\text{ is similar to } J_4(0) \oplus J_4(0). \end{aligned}$$

If $m = 5$, then we have:

$$\begin{aligned} (J_7(0))^5 &\text{ is similar to } J_2(0) \oplus J_2(0) \oplus J_1(0) \oplus J_1(0) \oplus J_1(0); \\ (J_8(0))^5 &\text{ is similar to } J_2(0) \oplus J_2(0) \oplus J_2(0) \oplus J_1(0) \oplus J_1(0). \end{aligned}$$

One notices immediately that the Jordan normal form of a Jordan block raised to the mth power consists of m blocks. The total dimension of these m blocks is equal to n and the sizes differ by at most one. □

Square roots of matrices in the complex indefinite inner product space were covered in the paper by Bolshakov et al. [4] and necessary and sufficient conditions for the existence of H-selfadjoint square roots of H-selfadjoint matrices over $\mathbb{C}$ can be found in the paper [18] by Van der Mee et al. Careful scrutiny of the relevant literature, however, yielded no results on mth roots of matrices in the complex indefinite inner product space. On the other hand, square roots of other special classes of matrices have been considered. For example, in [1] Alefeld and Schneider studied square roots of M-matrices while in [13] Fassbender et al. studied Hamiltonian square roots of skew-Hamiltonian matrices.

As mentioned in the statement of the research questions, there is a logical connection between square roots and polar decompositions of matrices. Any square matrix X admits a polar decomposition, that is, there exists a unitary matrix U and a positive semidefinite matrix A such that $X = UA$. The matrix A is uniquely determined as the positive semidefinite square root of the matrix X^*X and therefore the study of square roots can be invaluable in the study of polar decompositions.

1.2 Complex indefinite inner product space

We refer to the book by Gohberg, Lancaster and Rodman [14] for standard notation and terminology used in the thesis. We summarise the most relevant concepts here. The indefinite inner product, which is a function $[\cdot,\cdot]$ from $\mathbb{C}^n \times \mathbb{C}^n$ to $\mathbb{C}$, satisfies all the properties of a standard (definite) inner product, except for the positive semidefiniteness. To be more precise, the function $[\cdot,\cdot]$ is called an *indefinite inner product* in $\mathbb{C}^n$ if the following axioms are satisfied:

(i) linearity in the first argument: $[\alpha x_1 + \beta x_2, y] = \alpha[x_1, y] + \beta[x_2, y]$ for all $x_1, x_2, y \in \mathbb{C}^n$ and $\alpha, \beta \in \mathbb{C}$;

(ii) antisymmetry: $[x, y] = \overline{[y, x]}$ for all $x, y \in \mathbb{C}^n$;

(iii) nondegeneracy: if $[x, y] = 0$ for all $y \in \mathbb{C}^n$, then $x = 0$.

Therefore there can be a nonzero $x \in \mathbb{C}^n$ for which $[x, x]$ is negative or zero. As stated earlier, there exists a unique invertible Hermitian matrix $H \in \mathbb{C}^{n\times n}$ which generates the indefinite inner product. The H-adjoint of a matrix $A \in \mathbb{C}^{n\times n}$ is the unique $n \times n$ matrix $A^{[*]}$ such that $[Ax, y] = [x, A^{[*]}y]$ for all $x, y \in \mathbb{C}^n$. The matrix A is said to be *H-selfadjoint* if $A = A^{[*]}$ and *H-unitary* if A is invertible and $A^{-1} = A^{[*]}$. The notation Q_k is used for the $k \times k$ standard involutory permutation (sip) matrix with ones on the main anti-diagonal and zeros elsewhere.

The pairs of matrices of the form (A, H) where A is H-selfadjoint can be partitioned into equivalence classes under the relation of unitary similarity. Two pairs of matrices (A_1, H_1) and (A_2, H_2) are called *unitarily similar* (following the terminology of [14]) if there exists an invertible matrix $S \in \mathbb{C}^{n\times n}$ such that $A_2 = S^{-1}A_1S$ and $H_2 = S^*H_1S$. A unique representative, called the canonical form, for each of these equivalence classes can be found. The following theorem presents the *canonical form* of a pair (A, H) where A is H-selfadjoint.

Theorem 1.2.1 (Theorem 5.1.1, [14]). *Let $H \in \mathbb{C}^{n\times n}$ be an invertible Hermitian matrix and let $A \in \mathbb{C}^{n\times n}$ be an H-selfadjoint matrix. Then there exists an invertible matrix $S \in \mathbb{C}^{n\times n}$ such that $S^{-1}AS$ and S^*HS have the form*

$$\begin{aligned} S^{-1}AS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus \begin{bmatrix} J_{k_{\alpha+1}}(\lambda_{\alpha+1}) & 0 \\ 0 & J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\lambda_\beta) & 0 \\ 0 & J_{k_\beta}(\overline{\lambda}_\beta) \end{bmatrix}, \end{aligned} \tag{1.1}$$

where $\lambda_1, \ldots, \lambda_\alpha$ are real and $\lambda_{\alpha+1}, \ldots, \lambda_\beta$ are nonreal with positive imaginary parts, and

$$S^*HS = \varepsilon_1 Q_{k_1} \oplus \cdots \oplus \varepsilon_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \tag{1.2}$$

where $\varepsilon_1, \ldots, \varepsilon_\alpha$ are ± 1. For a given pair (A, H), where A is H-selfadjoint, the canonical form given by (1.1) *and* (1.2) *is unique up to a simultaneous permutation of corresponding diagonal blocks.*

In the canonical form given by (1.1) and (1.2), we say the block $J_{k_i}(\lambda_i)$ has *positive sign characteristic* if $\varepsilon_i = 1$ and *negative sign characteristic* if $\varepsilon_i = -1$.

An interesting subclass of the class of H-selfadjoint matrices is the class of H-nonnegative matrices. A matrix $A \in \mathbb{C}^{n\times n}$ is called *H-nonnegative* if $[Ax, x] \geq 0$ for all $x \in \mathbb{C}^n$. The H-nonnegative matrices have simple Jordan structures as can be seen in the following theorem.

Theorem 1.2.2 (Theorem 5.7.2, [14]). *A matrix $A \in \mathbb{C}^{n\times n}$ is H-nonnegative if and only if the following conditions hold:*

(i) *A is H-selfadjoint;*

(ii) *all the eigenvalues of A are real;*

(iii) *in the Jordan normal form of A, all Jordan blocks corresponding to the nonzero eigenvalues have size* 1*, and all Jordan blocks corresponding to the zero eigenvalue have size at most* 2*;*

(iv) *the Jordan block $J_{k_i}(\lambda_i)$ in the Jordan normal form of A has positive sign characteristic if $\lambda_i > 0$ and negative sign characteristic if $\lambda_i < 0$, and the Jordan blocks with eigenvalue zero and of size* 2 *have positive sign characteristic.*

Note that in the light of Theorem 1.2.1, the canonical form of a pair (A, H) where A is an H-nonnegative matrix, is given by

$$S^{-1}AS = \bigoplus_{i=1}^{q} J_1(\lambda_i) \oplus \bigoplus_{i=1}^{r-q} J_1(\lambda_{q+i}) \oplus \bigoplus_{i=1}^{s} J_1(0) \oplus \bigoplus_{i=1}^{t} J_2(0),$$

and

$$S^{*}HS = \bigoplus_{i=1}^{q} Q_1 \oplus \bigoplus_{i=1}^{r-q} (-Q_1) \oplus \bigoplus_{i=1}^{s} \varepsilon_i Q_1 \oplus \bigoplus_{i=1}^{t} Q_2,$$

where $\lambda_1, \ldots, \lambda_q > 0$, $\lambda_{q+1}, \ldots, \lambda_r < 0$, and $\varepsilon_i = \pm 1$.

The study of polar decompositions in indefinite inner product spaces was thoroughly covered by a series of papers by the authors Bolshakov, Van der Mee, Ran, Reichstein and Rodman, [4, 5, 6, 7, 18]. A matrix $X \in \mathbb{C}^{n\times n}$ is said to have an *H-polar decomposition* if there exists an H-unitary $U \in \mathbb{C}^{n\times n}$ and an H-selfadjoint $A \in \mathbb{C}^{n\times n}$ such that $X = UA$. Necessary and sufficient conditions for the existence of an H-polar decomposition in the complex case are found in the paper [7] by Bolshakov and Reichstein.

In the papers [19, 20] by Potapov, it was shown that if a matrix X over $\mathbb{C}$ is H-nonexpansive (that is, $[Xv, Xv] \leq [v, v]$ for all $v \in \mathbb{C}^n$), then X admits an H-polar decomposition $X = UA$ where A is H-selfadjoint with nonnegative eigenvalues. This result was generalized and extended to operators in the infinite dimensional case by Krein and Shmul'jan [17].

For easy reference we state here one of the main theorems in [4], which will be used later on.

Theorem 1.2.3 (Theorem 4.4, [4])**.** *An $n \times n$ complex matrix X admits an H-polar decomposition if and only if all the conditions below are satisfied.*

(i) *For each negative eigenvalue λ of $X^{[*]}X$ the part of the canonical form of $(X^{[*]}X, H)$ corresponding to λ can be presented in the form:*

$$\left(\bigoplus_{i=1}^{t} (J_{k_i}(\lambda) \oplus J_{k_i}(\lambda)), \bigoplus_{i=1}^{t} (Q_{k_i} \oplus -Q_{k_i}) \right).$$

(ii) *The part of the canonical form of $(X^{[*]}X, H)$ corresponding to the zero eigenvalue can be presented in the form:*

$$\left(\bigoplus_{i=0}^{m} B_i, \bigoplus_{i=0}^{m} H_i \right),$$

where $(B_0, H_0) = (0_{k_0\times k_0}, I_{p_0} \oplus -I_{n_0})$, $p_0 + n_0 = k_0$, *and where (for* $i = 1, \dots m$*) either*

$$(B_i, H_i) = (J_{k_i+1}(0) \oplus J_{k_i}(0),\ \eta_i Q_{k_i+1} \oplus \eta_i Q_{k_i}),$$

where $\eta_i = \pm 1$ *and* $k_i > 1$*, or*

$$(B_i, H_i) = (J_{k_i}(0) \oplus J_{k_i}(0),\ Q_{k_i} \oplus -Q_{k_i}),$$

where $k_i \geq 1$*.*

(iii) *Assume that (ii) holds. Let* ℓ_i *denote the size of a block* B_i*. There is a choice of basis* $\{e_{i,j}\}_{i=0}^{m}{}_{j=1}^{\ell_i}$ *in* $\mathbb{C}^n$ *which produces the canonical form in (ii) and*

$$\begin{aligned} \operatorname{Ker} X &= \operatorname{span}\{e_{i,1} + e_{i,k_i+1} \mid \ell_i = 2k_i, i = 1, \dots, m\} \\ &\oplus \operatorname{span}\{e_{i,1} \mid \ell_i = 2k_i - 1, i = 1, \dots, m\} \oplus \operatorname{span}\{e_{0,j}\}_{j=1}^{k_0}. \end{aligned}$$

The theory on Witt extensions established in [6] by Bolshakov et al. is a crucial step in the proof of the existence of H-polar decompositions. The next theorem, known as Witt's theorem, gives necessary conditions for the existence of a Witt extension. See also [7] by Bolshakov and Reichstein.

Theorem 1.2.4 (Theorem 2.1, [6]). *Let* $H_1, H_2 \in \mathbb{C}^{n\times n}$ *be invertible Hermitian matrices which define two indefinite inner products* $[\,\cdot\,,\cdot\,]_1$ *and* $[\,\cdot\,,\cdot\,]_2$ *on* $\mathbb{C}^n$*, respectively. Assume that* H_1 *and* H_2 *have the same number of positive eigenvalues. Let* $U_0 : V_1 \to V_2$ *be a nonsingular linear transformation, where* V_1 *and* V_2 *are subspaces in* $\mathbb{C}^n$*, such that*

$$[U_0 x, U_0 y]_2 = [x, y]_1 \quad \text{for every} \quad x, y \in V_1.$$

Then there exists a linear transformation $U : \mathbb{C}^n \to \mathbb{C}^n$ *such that*

$$[Ux, Uy]_2 = [x, y]_1 \quad \text{for every} \quad x, y \in \mathbb{C}^n \tag{1.3}$$

and

$$Ux = U_0 x \quad \text{for every} \quad x \in V_1. \tag{1.4}$$

Any linear transformation U satisfying (1.3) and (1.4) is called a *Witt extension* of U_0. To state an extended version of this theorem which includes a description of all Witt extensions, we first need some notation. Let the dimension of V_1 be equal to m and let $\{e_1, \dots, e_m\}$ be a basis of V_1 such that

$$[e_i, e_j]_1 = \begin{cases} 1 & \text{if } i = j = m_0 + 1, m_0 + 2, \dots, m_0 + m_+, \\ -1 & \text{if } i = j = m_0 + m_+ + 1, m_0 + m_+ + 2, \dots, m, \\ 0 & \text{otherwise,} \end{cases}$$

where $m_0 + m_+ + m_- = m$. Extend the basis for V_1 to a basis $\mathcal{E}$ for $\mathbb{C}^n$ as in the construction given in [6], and then form the matrix J_2 of size $n - m - m_0$ as the Gramian matrix of the last $n - m - m_0$ vectors in the basis $\mathcal{E}$.

Theorem 1.2.5 (Theorem 3.2, [6]). *Let $\tilde{U}$ be a Witt extension of the $n \times n$ matrix U_0 as in Theorem 1.2.4. Then there exists a J_2-unitary matrix P_1 (of size $n - m - m_0$), an $(n - m - m_0) \times m_0$ matrix P_2, and a skew-Hermitian $m_0 \times m_0$ matrix P_3, such that the matrix of $\tilde{U}$ has the form*

$$\tilde{U} = \begin{bmatrix} I_{m_0} & 0 & -\frac{1}{2}P_2^* J_2 P_2 + P_3 & -P_2^* J_2 P_1 \\ 0 & I_{m-m_0} & 0 & 0 \\ 0 & 0 & I_{m_0} & 0 \\ 0 & 0 & P_2 & P_1 \end{bmatrix}. \tag{1.5}$$

Here $m = \dim V_1$ and m_0 is the algebraic multiplicity of the zero eigenvalue of the Gramian matrix of any basis in V_1 with respect to $[\cdot, \cdot]_1$.

Conversely, if P_1 is an arbitrary J_2-unitary matrix of size $n - m - m_0$, P_2 is an arbitrary $(n - m - m_0) \times m_0$ matrix, and P_3 is an arbitrary skew-Hermitian $m_0 \times m_0$ matrix, then the matrix $\tilde{U}$ defined by (1.5) is a Witt extension of U_0.

Note that most of the results in this section are analogous for matrices over $\mathbb{R}$ except the canonical form for a pair of matrices (A, H) in Theorem 1.2.1, see for example [14].

1.3 Quaternion indefinite inner product space

The book by Leiba Rodman [22] provides us with the necessary basic theory of quaternion linear algebra. Every element in $\mathbb{H}$, the real skew field of quaternions, is of the form

$$x = x_0 + x_1\mathsf{i} + x_2\mathsf{j} + x_3\mathsf{k},$$

where $x_0, x_1, x_2, x_3 \in \mathbb{R}$ and the base vectors follow the following set of rules:

$$\mathsf{i}^2 = \mathsf{j}^2 = \mathsf{k}^2 = -1, \quad \mathsf{ij} = -\mathsf{ji} = \mathsf{k}, \quad \mathsf{jk} = -\mathsf{kj} = \mathsf{i}, \quad \mathsf{ki} = -\mathsf{ik} = \mathsf{j}.$$

One easily notices that multiplication in $\mathbb{H}$ is noncommutative and this is crucial to take into account when working with quaternions. Let the conjugate quaternion of $x \in \mathbb{H}$ be denoted by $\bar{x} = x_0 - x_1\mathsf{i} - x_2\mathsf{j} - x_3\mathsf{k}$.

The set of all $m \times n$ matrices in $\mathbb{H}$ is denoted by $\mathbb{H}^{m\times n}$ and it is considered as a left vector space. As can then be expected, an $n \times n$ quaternion matrix A has left eigenvalues and right eigenvalues which do not necessarily coincide. A nonzero vector $v \in \mathbb{H}^n$ is called a right (respectively, left) eigenvector of a matrix $A \in \mathbb{H}^{n\times n}$ corresponding to the right (respectively, left) eigenvalue $\lambda \in \mathbb{H}$ if $Av = v\lambda$ (respectively, $Av = \lambda v$) holds. It can be shown that A has exactly n right eigenvalues which are complex numbers with nonnegative imaginary parts, multiplicity taken into account, and all right eigenvalues of A are obtained from these n numbers since the spectrum of A is closed under similarity of quaternions. Thus, if λ is a right eigenvalue with right eigenvector v, then $\alpha^{-1}\lambda\alpha$ is also a right eigenvalue with right eigenvector $v\alpha$ for all nonzero $\alpha \in \mathbb{H}$. Throughout this thesis we shall work with right eigenvalues and hence we omit the word "right" and simply speak of eigenvalues.

It is well-known that there exists a complex matrix representation for quaternion matrices. This is achieved by a map $\omega_n : \mathbb{H}^{n\times n} \to \mathbb{C}^{2n\times 2n}$ defined as follows for a matrix $A \in \mathbb{H}^{n\times n}$ written as $A = A_1 + \mathrm{j}A_2$, where $A_1, A_2 \in \mathbb{C}^{n\times n}$:

$$\omega_n(A) = \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix}.$$

Moreover, this map ω_n is an isomorphism of the real algebra $\mathbb{H}^{n\times n}$ onto the real subalgebra Ω_{2n} of $\mathbb{C}^{2n\times 2n}$, where

$$\Omega_{2n} := \left\{ \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix} \mid A_1, A_2 \in \mathbb{C}^{n\times n} \right\}.$$

In the paper [2] by Alpay et al., basic classes of matrices including selfadjoint, unitary and plus matrices are studied in indefinite inner product spaces over the quaternions. The canonical form of a pair of quaternion matrices (A, H), where A is H-selfadjoint, can be found for example in the papers by Djokovic et al. and Sergeichuk [11, 23]. We state the canonical form here using the notation from [14].

Theorem 1.3.1 (Theorem 10.1.1, [22]). *Let $H \in \mathbb{H}^{n\times n}$ be an invertible Hermitian matrix and let $A \in \mathbb{H}^{n\times n}$ be an H-selfadjoint matrix. Then there exists an invertible matrix $S \in \mathbb{H}^{n\times n}$ such that*

$$\begin{aligned} S^{-1}AS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus \begin{bmatrix} J_{k_{\alpha+1}}(\lambda_{\alpha+1}) & 0 \\ 0 & J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\lambda_\beta) & 0 \\ 0 & J_{k_\beta}(\overline{\lambda}_\beta) \end{bmatrix}, \end{aligned} \tag{1.6}$$

where $\lambda_i \in \sigma(A) \cap \mathbb{R}$ for all $i = 1, \ldots, \alpha$, $\lambda_i \in \sigma(A) \cap \mathbb{C}_+$ for all $i = \alpha + 1, \ldots, \beta$, and

$$S^*HS = \varepsilon_1 Q_{k_1} \oplus \cdots \oplus \varepsilon_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \tag{1.7}$$

where $\varepsilon_i = \pm 1$. The canonical form $(S^{-1}AS,\ S^*HS)$ given by (1.6) and (1.7) is uniquely determined by the pair (A, H), up to a simultaneous permutation of corresponding diagonal blocks.

Polar decompositions in the standard inner product space over the skew field of quaternions were studied by Wiegmann [25]. In indefinite inner product spaces, however, no results on polar decompositions of quaternion matrices have been published.

1.4 Structure overview

The first part of the research, which is presented in Chapter 2, focuses on mth roots of H-selfadjoint matrices in the complex case. The case where $m = 2$ was covered in the paper by Bolshakov et al. [4], but see also the paper by Van der Mee et al. [18]. As in the square root case, the conditions for the existence of an H-selfadjoint mth root of an H-selfadjoint matrix, are only associated with negative eigenvalues and the eigenvalue zero.

Let B be a given H-selfadjoint matrix in $\mathbb{C}^{n\times n}$ where H is the invertible Hermitian matrix defining the indefinite inner product. The condition associated with negative eigenvalues states that, when m is even, in the canonical form of (B, H) the Jordan blocks with eigenvalue $\lambda < 0$ occur in pairs with opposite sign characteristic. Note that there are no restrictions to the existence of H-selfadjoint mth roots of H-selfadjoint matrices with negative eigenvalues in the case where m is odd. Now, the condition associated with the eigenvalue zero states that there exists a reordering of the *Segre characteristic* of B corresponding to the eigenvalue zero, i.e. a decreasing sequence of the sizes of the Jordan blocks of B with eigenvalue zero, such that when divided into m-tuples the difference between any two numbers in each m-tuple is at most one. This includes a somewhat complicated condition regarding the sign characteristic of the Jordan blocks with eigenvalue zero:

- If there is an even quantity of some number a in the kth m-tuple, then half of the Jordan blocks corresponding to that number a have positive sign characteristic (and the other half have negative sign characteristic);
- If there is an odd quantity of some number a in the kth m-tuple, say $2q + 1$, then either $q + 1$ of the Jordan blocks corresponding to that number a have positive sign characteristic (and the other q of the Jordan blocks have negative sign characteristic), or $q + 1$ of the Jordan blocks corresponding to that number a have negative sign characteristic (and the other q of the Jordan blocks have positive sign characteristic).

In the case where m is even and in an m-tuple the two numbers, say $a + 1$ and a, occur an odd number of times each, either both sets of Jordan blocks $J_{a+1}(0)$ and $J_a(0)$ have one more positive sign characteristic than the number of Jordan blocks with negative sign characteristic, or both sets have one more negative sign characteristic than the number of Jordan blocks with positive sign characteristic.

Let us illustrate the condition at the zero eigenvalue with an example.

Example 1.4.1. Let $m = 5$ and $B = \bigoplus_{i=1}^{5} J_3(0) \oplus \bigoplus_{i=1}^{4} J_2(0) \oplus J_1(0)$, so the Segre characteristic of B is $3, 3, 3, 3, 3, 2, 2, 2, 2, 1, 0, \ldots$. Suppose H is such that (B, H) is in canonical form. If we write

$$(3, 3, 3, 3, 3), (2, 2, 2, 2, 1),$$

then the first part of the condition associated with the zero eigenvalue is satisfied since this is a reordering of the Segre characteristic of B such that in each quintuple the difference between any two numbers is at most one. Note that there does not exist any other reordering of the Segre characteristic such that the condition is satisfied.

Turning to the second part of the condition, we look at each quintuple separately and count the numbers. In the first quintuple there are five 3s, i.e., an odd number of 3s, and $q = 2$ in the second point above. Thus for the condition to be satisfied, either $q + 1 = 3$ of the five Jordan blocks $J_a(0) = J_3(0)$ have positive sign characteristic and the other $q = 2$ have negative sign characteristic, or three of the $J_3(0)$ blocks have negative sign characteristic and the other two have positive sign characteristic. In the second quintuple there are four 2s and one 1. Thus half of the four $J_2(0)$ Jordan blocks (i.e. two) have positive sign characteristic and the other half (i.e. two) have negative sign characteristic, and the sign characteristic of the $J_1(0)$ Jordan block have either positive sign characteristic or negative sign characteristic. Once this is satisfied, the H-selfadjoint matrix B has an H-selfadjoint fifth root. □

Remarkably, as can be seen in Chapter 4, the results for this problem in the quaternion case are essentially the same as in the complex case. The reasons for this are the canonical form of a pair of quaternion matrices (A, H) where A is H-selfadjoint (as given in Theorem 1.3.1) and the fact that quaternion matrices have a complex matrix representation (given in (1.3)). See Chapter 4 for the proofs and note that they are presented for matrices in the subalgebra Ω_{2n} of $\mathbb{C}^{2n\times 2n}$. An explanation is included as to why that is sufficient for the goal of retrieving the results for quaternion matrices.

In Chapter 5 the main focus is on H-polar decompositions of matrices with quaternion entries. Necessary and sufficient conditions for the existence of an H-polar decomposition of a given quaternion matrix are obtained. It is important to note that these results are, once again, essentially the same as the results in the complex case. To understand why this research is a natural sequel to the H-selfadjoint mth roots of H-selfadjoint quaternion matrices we show here that the existence of H-selfadjoint square roots is a necessary condition for the existence of H-polar decompositions. Let X be any $n \times n$ quaternion matrix and suppose X admits an H-polar decomposition. Then we can write $X = UA$ for some H-unitary matrix U and some H-selfadjoint matrix A, ensuring the following

$$X^{[*]}X = (UA)^{[*]}UA = A^{[*]}U^{[*]}UA = AA = A^2.$$

Hence $X^{[*]}X$ has an H-selfadjoint square root A. In another useful result for the quaternion case, which is similar in the complex case, conditions are given for which $Y = U_0X$ is true for two linear transformations X and Y from $\mathbb{H}^n$ to $\mathbb{H}^m$ and where U_0 is an injective H-isometry in the indefinite inner product defined on $\mathbb{H}^m$ from $\operatorname{Im} X$ to $\operatorname{Im} Y$. Witt's theorem is proved for the quaternion case even though the proof is essentially the same as in the complex case, and it is used to extend the H-isometry U_0 to the whole space $\mathbb{H}^n$. This forms the essence of the sufficiency part of the proof for the existence of an H-polar decomposition, since we are provided with an H-unitary matrix in the H-polar decomposition. The necessary and sufficient conditions for the existence of an H-polar decomposition for a quaternion matrix X are then stated in the main theorem of Chapter 5 in terms of the canonical form of the pair $(X^{[*]}X, H)$ and a basis for the kernel of X. The first part of these conditions is related to the existence of an H-selfadjoint square root of $X^{[*]}X$, as we explained earlier. Note that although the work could also have been done for matrices in the subalgebra Ω_{2n} of $\mathbb{C}^{2n\times 2n}$ as in Chapter 4, we preferred a direct approach and proved the results for matrices in $\mathbb{H}^{n\times n}$.

The research recorded in Chapter 3 could be seen as a slight deviation from the rest of the thesis. It seemed compelling to study H-nonnegative matrices in the complex case because of the simple structure. Recall that H-nonnegative matrices have only real eigenvalues and their Jordan normal form is almost diagonal. Indeed, the Jordan blocks with nonzero eigenvalues have size 1 and the Jordan blocks with zero eigenvalue have size at most 2. Also, the Jordan blocks with positive (respectively, negative) eigenvalues have positive (respectively, negative) sign characteristic and the Jordan blocks of size 2 (with eigenvalue zero) have positive sign characteristic. Let B be an H-nonnegative complex matrix. Looking at the eigenvalue zero of the matrix B, we use the term Segre pairing to refer to a specific reordering, satisfying a particular set of rules, of the Segre characteristic. In the case where there exists a square root of B, the Segre pairing consists of pairs where each pair can only be one of the following:

$$(2,2), \quad (2,1), \quad (1,1), \quad \text{or} \quad (1,0).$$

The main idea of Chapter 3 is to separately study square roots of H-nonnegative complex matrices, and we first consider square roots of these matrices in general, then we look at H-selfadjoint square roots and finally study H-nonnegative square roots. Conditions are found for the existence of a specific square root (a general, H-selfadjoint or H-nonnegative square root) of B and are given mostly in terms of the numbers allowed in the Segre characteristic of B. For instance, an H-nonnegative matrix B has an H-nonnegative square root if and only if B has no negative eigenvalues and there are no 2s in the Segre characteristic of B corresponding to the eigenvalue zero, which essentially means that B is diagonalizable. An interesting part of this research is the description of the square roots in the nilpotent case. Once a square root exists, these results give the exact form of the (general, H-selfadjoint, H-nonnegative) square roots of B. The construction is again presented per pair in the Segre pairing of B, or more specifically the corresponding pairs of Jordan blocks with eigenvalue zero as in the canonical form of (B, H). In each case the canonical form of the pair (A, H), where A is a specific square root of B, is also given. Chapter 3 ends with a few results on the stability of H-nonnegative square roots of H-nonnegative matrices.

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Chapter 2

Complex H-selfadjoint mth roots[1]

Abstract. In this chapter necessary and sufficient conditions are given for the existence of an H-selfadjoint mth root of a given H-selfadjoint matrix. A construction is given of such an H-selfadjoint mth root when it does exist.

Keywords. Indefinite inner product space, H-selfadjoint matrices, Roots of matrices, Canonical forms.
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2.1 Introduction and Preliminaries

Let H be an invertible $n \times n$ Hermitian matrix. On $\mathbb{C}^n$ we consider the indefinite inner product generated by H, given by $[x, y] = \langle Hx, y\rangle$, where $\langle \cdot\,, \cdot\rangle$ denotes the standard inner product. Linear algebra in spaces with an indefinite inner product has been an area of active research over the past few decades, and many basic elements of the theory are summarised in [5]. An $n \times n$ matrix B is called H-selfadjoint if it is selfadjoint in the indefinite inner product given by H, or equivalently, if $HB = B^*H$. The problem studied in this chapter is that of finding H-selfadjoint mth roots of a given H-selfadjoint matrix B. This problem has been investigated in [1] for $m = 2$ where it plays a role in polar decompositions in an indefinite inner product space. Stability of H-selfadjoint square roots was studied in [17].

A matrix A is called an mth root of a matrix B if $A^m = B$. The problem of finding mth roots of a given matrix has been studied in the past; a first characterization can be found in the book by Wedderburn [18], and another characterization in [13]. In the book by Gantmacher [4] it is shown for the singular case that the function of taking mth roots can be applied to each Jordan block. Matrix mth roots have been studied extensively, see for example [2, 6, 15, 16].

Obviously, in the case where B is H-selfadjoint, a necessary condition for existence of an H-selfadjoint mth root is the existence of an mth root. Thus, this chapter will focus on the extra conditions needed for the existence of an H-selfadjoint mth root. In

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[17] existence and uniqueness of H-selfadjoint square roots of an H-selfadjoint matrix are studied, along with stability of such square roots when they exist.

More restrictive conditions on the H-selfadjoint square root can be imposed, for instance it is natural to impose the condition that the eigenvalues of A are in the open right half-plane, possibly including zero as well. In more generality than in the present setting such polar decompositions and square roots have been studied extensively in a sequence of papers by Higham, Mackey, Mackey, Mehl and Tisseur [7, 8, 11]. It turns out that imposing this extra condition on the eigenvalues of the square root leads to a square root which is unique and is computable using iterative methods. However, it restricts the class of matrices for which such a square root exists to those for which the structure of the zero eigenvalue is semisimple (if one includes the possibility of zero being an eigenvalue, but insists on uniqueness) or to those which are non-singular (if one insists on the eigenvalues of the square root lying in the open right half-plane). Square roots for other classes of structured matrices have been considered as well in [7, 8, 11]; see also [3] for the case of Hamiltonian square roots of skew-Hamiltonian matrices.

2.1.1 Notation

The notation $\langle \cdot , \cdot \rangle$ stands for the standard inner product in either $\mathbb{C}^n$ or $\mathbb{R}^n$, that is,

$$\langle x, y \rangle = \sum_{j=1}^{n} x_j \bar{y}_j,$$

where $x = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^T$, $y = \begin{bmatrix} y_1 & \cdots & y_n \end{bmatrix}^T \in \mathbb{C}^n$ or $\mathbb{R}^n$. The following definition and notation is taken from [5]. A function $[\,\cdot\,,\cdot\,]$ from $\mathbb{C}^n \times \mathbb{C}^n$ to $\mathbb{C}$ is called an *indefinite inner product* in $\mathbb{C}^n$ if it is linear in the first argument, anti-symmetric and nondegenerate. Therefore, the only possible difference with the standard inner product is that $[x, x]$ may be nonpositive for $x \neq 0$. Clearly, for every $n \times n$ invertible Hermitian matrix H (or real symmetric H) the formula $[x, y] = \langle Hx, y \rangle$, with $x, y \in \mathbb{C}^n$, defines an indefinite inner product on $\mathbb{C}^n$. Conversely, for any indefinite inner product $[\,\cdot\,,\cdot\,]$ on $\mathbb{C}^n$, there exists an invertible Hermitian matrix H such that $[x, y] = \langle Hx, y \rangle$ for all $x, y \in \mathbb{C}^n$.

The *H-adjoint* of a square matrix A, denoted by $A^{[*]}$, is the unique square matrix such that $[Ax, y] = [x, A^{[*]}y]$ for all $x, y \in \mathbb{C}^n$. Observe that $A^{[*]} = H^{-1}A^*H$.

We denote a single $n \times n$ Jordan block with eigenvalue $\lambda \in \mathbb{C}$ by:

$$J_n(\lambda) = \begin{bmatrix} \lambda & 1 & 0 & \cdots & 0 \\ 0 & \lambda & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \lambda & 1 \\ 0 & 0 & \cdots & 0 & \lambda \end{bmatrix}.$$

We will use the standard notation $\sigma(A)$ for the *spectrum* of A, that is, for the set of eigenvalues of a matrix A, including nonreal eigenvalues of real matrices. Furthermore, we denote by Q_n the $n \times n$ matrix with ones on the main anti-diagonal, which is called the backward identity matrix, or standard involutory permutation (sip) matrix.

We need the following well-known notation and result on Hermitian matrices. The *inertia* of a Hermitian matrix H is a triple consisting of the number of positive, negative and zero eigenvalues (counted with multiplicities), respectively, and will be denoted by $(i_+(H), i_-(H), i_0(H))$. According to Sylvester's law of inertia two Hermitian matrices have the same inertia if and only if they are congruent, see [10].

2.1.2 Important concepts

A subspace $\mathcal{M}$ of $\mathbb{C}^n$ is called *H-nondegenerate* if $x \in \mathcal{M}$ and $[x, y] = 0$ for all $y \in \mathcal{M}$ implies that $x = 0$. If $[x, y] = 0$ for all $x, y \in \mathcal{M}$, then $\mathcal{M}$ is called *H-neutral.*

A complex matrix A is *H-selfadjoint* if $A^{[*]} = A$, that is, if $HA = A^*H$. Thus, any H-selfadjoint matrix A is similar to A^*. If we consider, for example, a single Jordan block $J_n(\lambda)$ with real eigenvalue λ and if Q_n is as defined above, then $J_n(\lambda)$ is Q_n-selfadjoint. Furthermore, the spectrum $\sigma(A)$ of an H-selfadjoint matrix A is symmetric relative to the real axis. Also, the sizes of the Jordan blocks in the Jordan normal form of A with eigenvalue λ are equal to the sizes of the Jordan blocks with eigenvalue $\bar{\lambda}$. A proof of this result can be found in [5, Proposition 4.2.3].

A matrix A is called *H-unitary* if A is invertible and $A^{[*]} = A^{-1}$, i.e., $A^*HA = H$. The pairs (A_1, H_1) and (A_2, H_2) are said to be *unitarily similar* (following the terminology of [5]) if there exists an invertible matrix S such that $A_2 = S^{-1}A_1S$ and $H_2 = S^*H_1S$. If $H = H_1 = H_2$, then S is H-unitary and we say that A_1 and A_2 are *H-unitarily similar.* Note that if (A_1, H_1) and (A_2, H_2) are unitarily similar, it implies that A_1 is H_1-selfadjoint if and only if A_2 is H_2-selfadjoint.

If a matrix A is H-selfadjoint, then any power A^k of A is also H-selfadjoint since if we use $HA = A^*H$ repeatedly we have

$$HA^k = (HA)A^{k-1} = A^*HA^{k-1} = (A^*)^2HA^{k-2} = \cdots = (A^*)^kH = (A^k)^*H,$$

for any positive integer k.

2.1.3 Canonical form

The following theorem for the canonical form of H-selfadjoint matrices is taken from [1].

Theorem 2.1.1. *Let H be an invertible Hermitian $n \times n$ matrix over the field $\mathbb{C}$, and let A be an $n \times n$ H-selfadjoint matrix over $\mathbb{C}$. Then there exists an invertible $n \times n$ matrix S over $\mathbb{C}$ such that $S^{-1}AS$ and S^*HS have the form*

$$\begin{aligned} S^{-1}AS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus [J_{k_{\alpha+1}}(\lambda_{\alpha+1}) \oplus J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1})] \oplus \cdots \oplus [J_{k_\beta}(\lambda_\beta) \oplus J_{k_\beta}(\overline{\lambda}_\beta)], \end{aligned} \tag{2.1}$$

where $\lambda_1, \ldots, \lambda_\alpha$ are real and $\lambda_{\alpha+1}, \ldots, \lambda_\beta$ are nonreal with positive imaginary parts; and

$$S^*HS = \varepsilon_1 Q_{k_1} \oplus \cdots \oplus \varepsilon_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \tag{2.2}$$

where $\varepsilon_1, \ldots, \varepsilon_\alpha$ are ± 1. For a given pair (A, H), where A is H-selfadjoint, the canonical form (2.1) and (2.2) is unique up to permutation of orthogonal components in (2.2) and the same simultaneous permutation of the corresponding blocks in (2.1).

The theorem is well-known and can be traced back to Weierstrass and Kronecker, see for example Chapter 5 in [5], and the references given there.

The signs $\varepsilon_1, \ldots, \varepsilon_\alpha$ in (2.2) form the *sign characteristic* of the pair (A, H). Therefore, the sign characteristic consists of signs $+1$ or -1 attached to every partial multiplicity (equivalently, the size of a real Jordan block in the Jordan normal form) of A corresponding to a real eigenvalue. If $\varepsilon_i = 1$ (respectively, $\varepsilon_i = -1$) for some i, we say $\varepsilon_i Q_{k_i}$ is a *positive* (respectively, *negative*) *block* in S^*HS.

2.1.4 The main theorem

We need a definition and more notation before stating the main result. Recall the following definition from [14].

Definition 2.1.2. Let A be a square matrix with Jordan blocks $\bigoplus_{i=1}^{r} J_{n_i}(\lambda)$ at λ in its Jordan normal form and assume that $n_1 \geq n_2 \geq n_3 \geq \ldots \geq n_r > 0$. The *Segre characteristic* of A corresponding to the eigenvalue λ is defined as the sequence:

$$n_1, n_2, n_3, \ldots, n_r, 0, 0, \ldots.$$

Throughout the chapter this sequence will only be used when looking at the Jordan blocks associated with the eigenvalue zero. Let $n'_1, n'_2, \ldots, n'_{pm}, 0, \ldots$ be some reordering of the Segre characteristic of a nilpotent H-selfadjoint matrix B, where p is the number of nonzero m-tuples in this reordering. The kth m-tuple is

$$(n'_{m(k-1)+1}, n'_{m(k-1)+2}, \ldots, n'_{mk}).$$

Now let

$$\mathcal{B}_\nu^{(k)} := \{i \mid n'_i = \nu\,;\ m(k-1)+1 \leq i \leq mk\}, \tag{2.3}$$

so that $\left|\mathcal{B}_\nu^{(k)}\right|$ represents the number of blocks in H (or A) of size ν which corresponds to the kth m-tuple, that is, $k = 1, \ldots, p$ and ν can be any number in the Segre characteristic of B.

Let us partition the canonical form (J, H_B) of (B, H) as follows:

$$J = J_0 \oplus J_1 \oplus J_2 \quad \text{and} \quad H_B = H_0 \oplus H_1 \oplus H_2,$$

where J_0 is a direct sum of blocks of the form $J_{k_j}(0)$ for some k_j, J_1 is a direct sum of blocks of the form $J_{k_j}(\alpha_j)$ for some k_j and $\alpha_j < 0$, and J_2 is a matrix in Jordan normal form with all eigenvalues not in $(-\infty, 0]$, and where the matrices H_0, H_1 and H_2 correspond to the matrices J_0, J_1 and J_2.

In the next section, the search for necessary and sufficient conditions for existence of an H-selfadjoint mth root is reduced to the treatment of the same problem for the pairs (J_0, H_0), (J_1, H_1) and (J_2, H_2) separately. These cases are then studied, and the results are summarised in the following main theorem. In addition, for each of these cases, in the next section an explicit construction is given in the case that an H-selfadjoint mth root exists.

Theorem 2.1.3. *Let B be an H-selfadjoint matrix. Then there exists an H-selfadjoint matrix A such that $A^m = B$ if and only if the canonical form of (B, H), given by (J, H_B), has the following properties:*

1. *There exists a reordering,* $n'_1, n'_2, \ldots, n'_{pm}, 0, \ldots$, *of the Segre characteristic corresponding to the zero eigenvalue of* B *such that for all* k *the* m*-tuple*

$$(n'_{m(k-1)+1}, \ldots, n'_{mk})$$

is descending and the difference between $n'_{m(k-1)+1}$ *and* n'_{mk} *is at most one.*

2. *For some reordering satisfying the first property, the number of positive blocks in* H_0 *of size* ν *is equal to* $\sum_{k=1}^{p} \pi_{\nu,k}$ *where*

$$\pi_{\nu,k} = \begin{cases} \frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right|\right) & \text{if } \left|\mathcal{B}_\nu^{(k)}\right| \text{ is even} \\ \frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right| + \eta_k\right) & \text{if } \left|\mathcal{B}_\nu^{(k)}\right| \text{ is odd} \end{cases},$$

with η_k *either equal to* 1 *or* -1.

3. *The blocks in* J_1 *and* H_1 *for an even* m*, can be reordered in the following way:*

$$J_1 = \bigoplus_{j=1}^{t} \left(J_{k_j}(\alpha_j) \oplus J_{k_j}(\alpha_j)\right) \quad \text{and} \quad H_1 = \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus (-Q_{k_j})\right).$$

2.2 Existence of an H-selfadjoint mth root

Given an H-selfadjoint matrix B, we are interested in finding H-selfadjoint mth roots of B, if they exist. It is well-documented (for example in [9, p. 461]) that for finding mth roots, one may limit oneself to finding the mth root of the Jordan normal form of any matrix. We show that the same is true for finding H-selfadjoint mth roots.

Consider the following result which implies that it is sufficient to start with the pair (B, H) in canonical form. It shows how mth roots of matrices which are part of pairs in the same equivalent class are related.

Lemma 2.2.1. *Let the pair* (X, H_X) *be unitarily similar to the pair* (Y, H_Y) *where* H_X *and* H_Y *are invertible Hermitian matrices, that is, there exists an invertible matrix* P *such that*

$$P^{-1}XP = Y, \quad \text{and} \quad P^*H_XP = H_Y. \tag{2.4}$$

Let the matrix $\tilde{A}$ *be an* H_X*-selfadjoint* m*th root of* X*. Then the matrix* $A := P^{-1}\tilde{A}P$ *is an* H_Y*-selfadjoint* m*th root of* Y.

Proof. Suppose that the equalities in (2.4) hold. Let the matrix $\tilde{A}$ be an H_X-selfadjoint matrix such that $\tilde{A}^m = X$. Then by writing $(P^{-1}\tilde{A}P)^m = P^{-1}\tilde{A}^mP = Y$, we obtain an mth root $A := P^{-1}\tilde{A}P$ of Y. It follows that $(\tilde{A}, H_X)$ and (A, H_Y) are unitarily similar and therefore the mth root A is H_Y-selfadjoint. □

The above lemma can be used in the proofs for the existence of an H-selfadjoint mth root of a given B, where we only need to construct a matrix $\tilde{A}$ whose mth power has Jordan normal form equal to B and check that there exists an invertible matrix P such that equations (2.4) hold.

From the literature (for example [9, p. 461]) we also know that when finding mth roots of a matrix B in Jordan normal form, we may consider blocks with each eigenvalue separately. The situation is a bit more complicated in the case of H-selfadjoint mth roots, because of the restriction placed by the canonical form as given in Theorem 2.1.1. We therefore need to group the blocks in B in pairs of complex conjugate eigenvalues, except in the case where the eigenvalue is real, in which case it may appear on its own, see also [1] for the case of finding H-selfadjoint square roots. We discuss the existence of H-selfadjoint mth roots for the cases where B has only positive real eigenvalues, only nonreal eigenvalues, only eigenvalue zero, and only negative eigenvalues separately in the next few subsections.

Note that although functional calculus can be used for the case where B has neither negative nor zero eigenvalues, we prefer to give a detailed proof using only linear algebra techniques.

2.2.1 The case where B has only positive eigenvalues

In this subsection we find conditions for the existence of an H-selfadjoint mth root of an H-selfadjoint matrix which has only positive real numbers as eigenvalues. We start with a discussion which leads to the main result of this subsection.

Let $B = J_n(\lambda)$ and $H = \varepsilon Q_n$, where $\varepsilon = \pm 1$ and λ is a positive real number. Let $\tilde{A} = J_n(\mu)$, where μ is the positive real mth root of λ. Then the Jordan normal form of $\tilde{A}^m$ is equal to B. Note that the matrix $\tilde{A}$ is H_A-selfadjoint where $H_A = \delta Q_n$, for $\delta = 1$ or $\delta = -1$. Take $\delta = \varepsilon$. Next, we construct an invertible matrix P such that the equations

$$P^{-1}\tilde{A}^m P = B \quad \text{and} \quad P^* H_A P = H \tag{2.5}$$

hold and then Lemma 2.2.1 can be applied. Therefore, we examine the structure of the matrix $P^* H_A P$ where the columns of P form a Jordan basis for the matrix $\tilde{A}^m$. Recall that, see for example [12, p. 594], the matrix P will be of the form

$$P = \begin{bmatrix} (\tilde{A}^m - \lambda I)^{n-1} y & \cdots & (\tilde{A}^m - \lambda I) y & y \end{bmatrix}, \tag{2.6}$$

where $y = (y_1, \ldots, y_n)^T \in \operatorname{Ker}(\tilde{A}^m - \lambda I)^n$ but $y \notin \operatorname{Ker}(\tilde{A}^m - \lambda I)^{n-1}$. Note that in this case $\operatorname{Ker}(\tilde{A}^m - \lambda I)^n = \mathbb{C}^n$.

We write $p_i = (\tilde{A}^m - \lambda I)^{n-i} y$ and let the entries of the matrix $P^* H_A P$ be denoted by $\phi_{i,j}(y)$. Then, see for example the proof of Theorem 2.1.1 in [5], the matrix $P^* H_A P$ is an anti-lower triangular Hankel matrix and can be uniquely determined by using only the n values in its last row. Therefore $P^* H_A P = H$ if and only if

$$\phi_j(y) := \phi_{n,j}(y) = [p_j, p_n] = y^* H_A (\tilde{A}^m - \lambda I)^{n-j} y = \begin{cases} 1 & \text{if } j = 1, \\ 0 & \text{if } j = 2, \ldots, n. \end{cases} \tag{2.7}$$

Since the matrix $(\tilde{A}^m - \lambda I)$ is upper triangular with zeros on the diagonal, the matrix $(\tilde{A}^m - \lambda I)^{n-j}$ will have zeros in the first $n - j$ columns and in the last $n - j$ rows. This implies that the entry $\phi_j(y) = \phi_{n,j}(y) = y^* H_A (\tilde{A}^m - \lambda I)^{n-j} y$ for each $j = 1, \ldots, n$, is an expression in the variables $y_n, \ldots, y_{n-j+1}$, that is,

$$\begin{aligned}
\phi_1(y) &= \phi_1(y_n) \\
\phi_2(y) &= \phi_2(y_n, y_{n-1}) \\
\phi_3(y) &= \phi_3(y_n, y_{n-1}, y_{n-2}) \\
&\vdots \\
\phi_n(y) &= \phi_n(y_n, \ldots, y_1),
\end{aligned}$$

where each one is a sum of terms of the form $c\bar{y}_i y_j$, $c \in \mathbb{R}$, see Example 2.2.2.

Hence, using the first equation in (2.7) to find the nth entry in y and the other equations in (2.7) to write each of the other entries in y in terms of the nth entry, we construct the vector y and consequently find a matrix P using (2.6) such that equations (2.5) hold. It now follows from Lemma 2.2.1 that the matrix $A := P^{-1}\tilde{A}P$ is an H-selfadjoint mth root of B.

The procedure is illustrated in the following example.

Example 2.2.2. Let $B = J_3(\lambda)$ where λ is a positive real number and let $\tilde{A} = J_3(\mu)$ where μ is the positive real mth root of λ. The matrix B is H-selfadjoint where $H = Q_3$ and the matrix $\tilde{A}$ is H_A-selfadjoint where $H_A = H = Q_3$. Then the Jordan normal form of

$$\tilde{A}^m = \begin{bmatrix} \lambda & m\mu^{m-1} & \frac{1}{2}m(m-1)\mu^{m-2} \\ 0 & \lambda & m\mu^{m-1} \\ 0 & 0 & \lambda \end{bmatrix}$$

is B and therefore we know that the invertible matrix P for which the equality $P^{-1}\tilde{A}^m P = B$ is true, will be of the form

$$\begin{aligned}
P &= \begin{bmatrix} (\tilde{A}^m - \lambda I)^2 y & (\tilde{A}^m - \lambda I)y & y \end{bmatrix} \\
&= \begin{bmatrix} (m\mu^{m-1})^2 y_3 & m\mu^{m-1}y_2 + \frac{1}{2}m(m-1)\mu^{m-2}y_3 & y_1 \\ 0 & m\mu^{m-1}y_3 & y_2 \\ 0 & 0 & y_3 \end{bmatrix},
\end{aligned}$$

where $y = (y_1, y_2, y_3)^T \in \text{Ker } (\tilde{A}^m - \lambda I)^3 = \mathbb{C}^3$ but $y \notin \text{Ker } (\tilde{A}^m - \lambda I)^2$. Then by equating the entries in the third row, $P^*HP = H$ holds if and only if the following equations hold:

$$\begin{aligned}
1 = \quad & \phi_1(y_3) && = (m\mu^{m-1})^2 \bar{y}_3 y_3, \\
0 = \quad & \phi_2(y_3, y_2) && = m\mu^{m-1}\bar{y}_2 y_3 + \frac{1}{2}m(m-1)\mu^{m-2}\bar{y}_3 y_3 + m\mu^{m-1}\bar{y}_3 y_2, \\
0 = \quad & \phi_3(y_3, y_2, y_1) && = \bar{y}_1 y_3 + \bar{y}_2 y_2 + \bar{y}_3 y_1.
\end{aligned}$$

Assume that y is real, then we can solve the first equation for y_3, choose the positive value and substitute into the second equation to find y_2, and lastly, solve the third equation for y_1. Therefore, one solution to these equations is as follows:

$$y_1 = \frac{-(m-1)^2}{32m\mu^{m+1}}; \quad y_2 = \frac{-(m-1)}{4m\mu^m}; \quad y_3 = \frac{1}{m\mu^{m-1}}. \quad \square$$

In the case where B consists of more than one block, the construction may be applied to each block separately. We have thus proved the following theorem.

Theorem 2.2.3. *Let B be an H-selfadjoint matrix with a spectrum consisting only of positive real numbers. Then there exists an H-selfadjoint matrix A such that $A^m = B$.*

2.2.2 The case where B has only nonreal eigenvalues

In this subsection we give a proof for the existence of an H-selfadjoint mth root in the case where B has only nonreal eigenvalues.

Theorem 2.2.4. *Let B be an H-selfadjoint matrix with a spectrum consisting only of nonreal numbers. Then there exists an H-selfadjoint matrix A such that $A^m = B$.*

Proof. Let B be a $2n \times 2n$ H-selfadjoint matrix with nonreal eigenvalues. Assume that the pair (B, H) is in canonical form and that B has only one number and its complex conjugate as eigenvalues, each with a geometric multiplicity of one. Thus, with λ being a nonreal number,

$$B = J_n\big(\lambda\big) \oplus J_n\left(\bar{\lambda}\right) \quad \text{and} \quad H = Q_{2n}.$$

Let μ be any mth root of λ and

$$\tilde{A} = J_n\left(\mu\right) \oplus J_n\left(\bar{\mu}\right),$$

then the Jordan normal form of $\tilde{A}^m$ is equal to B. Note that the matrix $\tilde{A}$ is H_A-selfadjoint where $H_A = Q_{2n}$. We once again construct a $2n \times 2n$ invertible matrix P such that $P^{-1}\tilde{A}^m P = B$ and $P^* H_A P = H$ hold. For the first equality to hold, the columns of P have to form a Jordan basis for the matrix $\tilde{A}^m$, and therefore $P = P_1 \oplus P_2$ where

$$P_1 = \left[\big((J_n(\mu))^m - \lambda I\big)^{n-1} y \quad \cdots \quad y\right]$$

and

$$P_2 = \left[\big((J_n(\bar{\mu}))^m - \bar{\lambda} I\big)^{n-1} z \quad \cdots \quad z\right],$$

where $y \in \operatorname{Ker}\left((J_n(\mu))^m - \lambda I\right)^n = \mathbb{C}^n$ but $y \notin \operatorname{Ker}\left((J_n(\mu))^m - \lambda I\right)^{n-1}$, and where $z \in \operatorname{Ker}\left((J_n(\bar{\mu}))^m - \bar{\lambda} I\right)^n = \mathbb{C}^n$ but $z \notin \operatorname{Ker}\left((J_n(\bar{\mu}))^m - \bar{\lambda} I\right)^{n-1}$. Take $z = \bar{y}$, i.e. $P_2 = \overline{P_1}$. Then, by a simple calculation, one finds that $P^* H_A P = H$ if and only if $P_1^T Q_n P_1 = Q_n$, and by following a similar process as in Section 2.2.1, one can see that this is true if and only if

$$\phi_j(y) = \phi_{n,j}(y) = y^T Q_n((J_n(\mu))^m - \lambda I)^{n-j} y = \begin{cases} 1 & \text{if } j = 1, \\ 0 & \text{if } j = 2, \ldots, n. \end{cases}$$

Note that, similarly to the case in Section 2.2.1, each $\phi_j(y)$ is an expression in the variables $y_n, \ldots, y_{n-j+1}$, and a solution to these equations can be found by solving the first equation for y_n and substituting back into the other equations. Therefore, there exists a solution to $P^* H_A P = H$ which also satisfies $P^{-1}\tilde{A}^m P = B$, and hence by Lemma 2.2.1, the matrix $A := P^{-1}\tilde{A}P$ is an H-selfadjoint mth root of B. In the case where B consists of more than one pair of blocks, the construction can be applied to each pair of blocks separately. □

2.2.3 The case where B has only eigenvalue zero

In this section we consider the case where B has only zero in its spectrum, so that B is nilpotent. Obviously the mth roots of B will then be nilpotent as well.

The main theorem concerning H-selfadjoint mth roots in this case is given. The first property is necessary for the existence of an mth root in general and this is well-known (see for example [9, Theorem 6.4.12]).

Theorem 2.2.5. *Let B be a nilpotent H-selfadjoint matrix. Then there exists an H-selfadjoint matrix A such that $A^m = B$ if and only if the canonical form of (B, H), given by (J, H_B), has the following properties:*

1. *There exists a reordering, $n'_1, n'_2, n'_3, \ldots, n'_{pm}, 0, \ldots,$ of the Segre characteristic of B such that for all k the m-tuple $(n'_{m(k-1)+1}, \ldots, n'_{mk})$ is descending and the difference between $n'_{m(k-1)+1}$ and n'_{mk} is at most one.*

2. *For some reordering satisfying the first property, the number of positive blocks in H_B of size ν is equal to $\sum_{k=1}^{p} \pi_{\nu,k}$ where*

$$\pi_{\nu,k} = \begin{cases} \frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right|\right) & \text{if } \left|\mathcal{B}_\nu^{(k)}\right| \text{ is even,} \\ \frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right| + \eta_k\right) & \text{if } \left|\mathcal{B}_\nu^{(k)}\right| \text{ is odd,} \end{cases} \tag{2.8}$$

   with η_k either equal to 1 or -1.

The proof will follow after some results and two examples.

Lemma 2.2.6. *Let the matrix A be equal to $J_n(0)$. Then A^m has Jordan normal form*

$$\bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0), \tag{2.9}$$

where $n = am + r$, for $a, r \in \mathbb{Z}$, $0 < r \leq m$.

Note that if $m \geq n$, then $a = 0$ and $r = n$, that is, (2.9) is equal to $\bigoplus_{i=1}^{n} J_1(0)$, which is the $n \times n$ zero matrix.

Proof. Let $A = J_n(0)$. If $m \geq n$, then $A^m = (J_n(0))^m = 0 = \bigoplus_{i=1}^{n} J_1(0)$. Let $m < n$, then by raising A to the mth power, we have

$$A^m = \begin{bmatrix} 0 & \cdots & 0 & 1 & & \\ & \ddots & & \ddots & \ddots & \\ & & \ddots & & \ddots & 1 \\ & & & \ddots & & 0 \\ & & & & \ddots & \vdots \\ & & & & & 0 \end{bmatrix},$$

where the one in the first row is in the $(m+1)$th column. It can easily be seen that the Jordan chains of A^m are

$$\begin{aligned} C_1 &= \{e_i \mid i \equiv 1 \,(\mathrm{mod}\ m);\ i = 1, \ldots, n\}, \\ C_2 &= \{e_i \mid i \equiv 2 \,(\mathrm{mod}\ m);\ i = 1, \ldots, n\}, \\ \vdots\ \ & \qquad \vdots \\ C_{m-1} &= \{e_i \mid i \equiv m-1 \,(\mathrm{mod}\ m);\ i = 1, \ldots, n\}, \\ C_m &= \{e_i \mid i \equiv 0 \,(\mathrm{mod}\ m);\ i = 1, \ldots, n\}. \end{aligned} \tag{2.10}$$

Use the division algorithm to write $n = am + r$ where $a, r \in \mathbb{Z}$, $0 < r \leq m$. Then the number of elements in each set C_j is

$$|C_j| = \begin{cases} a+1 & \text{for } 1 \leq j \leq r, \\ a & \text{for } r+1 \leq j \leq m. \end{cases} \tag{2.11}$$

Let S be the $n \times n$ invertible matrix with columns consisting of the vectors in the Jordan chains $C_1, \ldots, C_m$. Then, since the lengths of Jordan chains coincide with the sizes of the corresponding Jordan blocks and by using (2.11), we have the Jordan normal form of A^m:

$$S^{-1}A^mS = \bigoplus_{j=1}^{m} J_{|C_j|}(0) = \bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0). \qquad \square$$

An interesting corollary that we obtain from this result, is the following.

Corollary 2.2.7. *If the number of Jordan blocks with eigenvalue zero of a matrix B is not divisible by m and there are no $J_1(0)$ blocks, that is, no entry in the Segre characteristic of B corresponding to the zero eigenvalue is equal to one, then B does not have an mth root.*

The following result shows the relation between the canonical forms as will be illustrated in the examples.

Lemma 2.2.8. *The pair (A, H) has canonical form $(J_n(0), \eta Q_n)$, $\eta = \pm 1$, if and only if (A^m, H) has canonical form*

$$\left(\bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0),\ \bigoplus_{i=1}^{r} \varepsilon_i Q_{a+1} \oplus \bigoplus_{i=1}^{m-r} \varepsilon_{r+i} Q_a \right),$$

where the signs are as follows: If r (respectively $m-r$) is even, the number of signs ε_i, where $i = 1, \ldots, r$ (respectively $i = r+1, \ldots, m$), which are equal to η is $\frac{r}{2}$ (respectively $\frac{m-r}{2}$). If r (respectively $m-r$) is odd, the number of signs ε_i, where $i = 1, \ldots, r$ (respectively $i = r+1, \ldots, m$), which are equal to η is $\frac{r+1}{2}$ (respectively $\frac{m-r+1}{2}$). In both cases the rest of the signs are equal to $-\eta$.

The next two examples illustrate much of the general case to be proved after the examples.

Example 2.2.9. Let the matrix

$$B = \bigoplus_{i=1}^{3} J_4(0) \oplus \bigoplus_{i=1}^{7} J_3(0) \oplus \bigoplus_{i=1}^{2} J_2(0)$$

be H-selfadjoint where

$$H = \bigoplus_{i=1}^{3} \varepsilon_i Q_4 \oplus \bigoplus_{i=1}^{7} \varepsilon_{3+i} Q_3 \oplus \bigoplus_{i=1}^{2} \varepsilon_{10+i} Q_2$$

for some $\varepsilon_j = \pm 1$. B has Segre characteristic $4,4,4,3,3,3,3,3,3,3,2,2,0,\ldots$. We wish to determine for which values of ε_j the matrix B would have an H-selfadjoint fourth root. Thus, in terms of notation of Theorem 2.1.3, $n = 37$ and $m = 4$. For the purpose of this example, we just consider the following grouping of the Segre characteristic into 4-tuples:

$$(4,4,4,3),(3,3,3,3),(3,3,2,2),(0,0,0,0),\ldots. \tag{2.12}$$

Then $p = 3$ with p as in Theorem 2.1.3. The other possible reorderings of the Segre characteristic are

$$(4,4,3,3),(4,3,3,3),(3,3,2,2),(0,0,0,0),\ldots \text{ and}$$

$$(4,4,4,3),(3,3,3,2),(3,3,3,2),(0,0,0,0),\ldots.$$

Any fourth root of B will be similar to $A = \bigoplus_{j=1}^{q} J_{n_j}(0)$ for some integers q and n_j, since it will also be nilpotent. If $n_j = 4a_j + r_j$ for some $a_j, r_j \in \mathbb{Z}$, $0 < r_j \leq 4$, then by Lemma 2.2.6, we have that A^4 has Jordan normal form

$$\bigoplus_{j=1}^{q} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=1}^{4-r_j} J_{a_j}(0) \right). \tag{2.13}$$

We also know that A^4 is similar to B and therefore we know the number of blocks of size 4, 3 and 2 in (2.13). If we restrict ourselves to the ordering (2.12), it can easily be seen that $a_1 = 3$, $r_1 = 3$, $a_2 = 2$, $r_2 = 4$, $a_3 = 2$ and $r_3 = 2$, which then give the values $n_1 = 15$, $n_2 = 12$ and $n_3 = 10$ from the division algorithm. Compare with the exercises 6.4.10-6.4.13 in [9]. Hence, using the ordering (2.12), any fourth root of B will have the form $A = J_{15}(0) \oplus J_{12}(0) \oplus J_{10}(0)$. By Theorem 2.1.1, the pair (A, H_A) is in canonical form, with $H_A = \eta_1 Q_{15} \oplus \eta_2 Q_{12} \oplus \eta_3 Q_{10}$ for some $\eta_1 = \pm 1$, $\eta_2 = \pm 1$ and $\eta_3 = \pm 1$. We wish to find a fourth root (which is similar to A) that is H-selfadjoint and to this end we construct a matrix P satisfying (2.4) where $X = A^4$, $Y = B$, $H_X = H_A$ and $H_Y = H$. Write down the Jordan chains of the matrix A^4 by using the notation in (2.10) adapted for more blocks:

$C_1 = \{e_1, e_5, e_9, e_{13}\},\ C_2 = \{e_2, e_6, e_{10}, e_{14}\},\ C_3 = \{e_3, e_7, e_{11}, e_{15}\},\ C_4 = \{e_4, e_8, e_{12}\};$
$C_{16} = \{e_{16}, e_{20}, e_{24}\},\ C_{17} = \{e_{17}, e_{21}, e_{25}\},\ C_{18} = \{e_{18}, e_{22}, e_{26}\},\ C_{19} = \{e_{19}, e_{23}, e_{27}\};$
$C_{28} = \{e_{28}, e_{32}, e_{36}\},\ C_{29} = \{e_{29}, e_{33}, e_{37}\},\ C_{30} = \{e_{30}, e_{34}\},\ C_{31} = \{e_{31}, e_{35}\}.$

Note that the matrix having these Jordan chains as columns does not satisfy the equations (2.4), since the only Jordan chains spanning H_A-nondegenerate spaces are C_2 and C_4. All the other Jordan chains span H_A-neutral spaces. Therefore, a change of basis is necessary on these Jordan chains to ensure that all Jordan chains in the new basis span H_A-nondegenerate spaces. This is done in the following way: let P be the invertible 37×37 matrix whose columns consist of the following (new) Jordan chains:

$$\begin{aligned}
C_1^+ &= \{(e_1+e_3)/\sqrt{2}, (e_5+e_7)/\sqrt{2}, (e_9+e_{11})/\sqrt{2}, (e_{13}+e_{15})/\sqrt{2}\},\\
C_2 &= \{e_2, e_6, e_{10}, e_{14}\},\\
C_1^- &= \{(e_1-e_3)/\sqrt{2}, (e_5-e_7)/\sqrt{2}, (e_9-e_{11})/\sqrt{2}, (e_{13}-e_{15})/\sqrt{2}\},\\
C_4 &= \{e_4, e_8, e_{12}\},\\
C_{16}^+ &= \{(e_{16}+e_{19})/\sqrt{2}, (e_{20}+e_{23})/\sqrt{2}, (e_{24}+e_{27})/\sqrt{2}\},\\
C_{17}^+ &= \{(e_{17}+e_{18})/\sqrt{2}, (e_{21}+e_{22})/\sqrt{2}, (e_{25}+e_{26})/\sqrt{2}\},\\
C_{17}^- &= \{(e_{17}-e_{18})/\sqrt{2}, (e_{21}-e_{22})/\sqrt{2}, (e_{25}-e_{26})/\sqrt{2}\},\\
C_{16}^- &= \{(e_{16}-e_{19})/\sqrt{2}, (e_{20}-e_{23})/\sqrt{2}, (e_{24}-e_{27})/\sqrt{2}\},\\
C_{28}^+ &= \{(e_{28}+e_{29})/\sqrt{2}, (e_{32}+e_{33})/\sqrt{2}, (e_{36}+e_{37})/\sqrt{2}\},\\
C_{28}^- &= \{(e_{28}-e_{29})/\sqrt{2}, (e_{32}-e_{33})/\sqrt{2}, (e_{36}-e_{37})/\sqrt{2}\},\\
C_{30}^+ &= \{(e_{30}+e_{31})/\sqrt{2}, (e_{34}+e_{35})/\sqrt{2}\},\\
C_{30}^- &= \{(e_{30}-e_{31})/\sqrt{2}, (e_{34}-e_{35})/\sqrt{2}\}.
\end{aligned}$$

Then $P^{-1}A^4P = B$ holds, and comparison of entries in P^*H_AP and H gives us the relationship between the signs of ε_j for $j = 1, \ldots, 12$ and those of η_j for $j = 1, 2, 3$. In order to determine which combinations of ε_j could rise to H-selfadjoint B with H-selfadjoint fourth roots, we consider all eight combinations of η_j and determine the possible values of ε_j that would correspond to these η_j for each of the blocks associated with the 4-tuples in (2.12).

Consider Table 2.1 which gives the signs of the blocks $Q_{n_i'}$ in H corresponding to each entry n_i' in the Segre characteristic of B by specifying η_j from H_A.

4-tuples			4	4	4	3	3	3	3	3	3	3	2	2
	ε_i		ε_1	ε_2	ε_3	ε_4	ε_5	ε_6	ε_7	ε_8	ε_9	ε_{10}	ε_{11}	ε_{12}
η_1	η_2	η_3	$+\eta_1$	$+\eta_1$	$-\eta_1$	$+\eta_1$	$+\eta_2$	$+\eta_2$	$-\eta_2$	$-\eta_2$	$+\eta_3$	$-\eta_3$	$+\eta_3$	$-\eta_3$
1	1	1	$+$	$+$	$-$	$+$	$+$	$+$	$-$	$-$	$+$	$-$	$+$	$-$
1	1	-1	$+$	$+$	$-$	$+$	$+$	$+$	$-$	$-$	$-$	$+$	$-$	$+$
1	-1	1	$+$	$+$	$-$	$+$	$-$	$-$	$+$	$+$	$+$	$-$	$+$	$-$
1	-1	-1	$+$	$+$	$-$	$+$	$-$	$-$	$+$	$+$	$-$	$+$	$-$	$+$
-1	1	1	$-$	$-$	$+$	$-$	$+$	$+$	$-$	$-$	$+$	$-$	$+$	$-$
-1	1	-1	$-$	$-$	$+$	$-$	$+$	$+$	$-$	$-$	$-$	$+$	$-$	$+$
-1	-1	1	$-$	$-$	$+$	$-$	$-$	$-$	$+$	$+$	$+$	$-$	$+$	$-$
-1	-1	-1	$-$	$-$	$+$	$-$	$-$	$-$	$+$	$+$	$-$	$+$	$-$	$+$

Table 2.1: Signs of all ε_i corresponding to each combination of η_j

To explain Table 2.1, we look at the first row which shows that if η_1, η_2 and η_3 are all equal to $+1$, then we have that $\varepsilon_1 = \varepsilon_2 = \varepsilon_4 = \varepsilon_5 = \varepsilon_6 = \varepsilon_9 = \varepsilon_{11} = +1$ and

$\varepsilon_3 = \varepsilon_7 = \varepsilon_8 = \varepsilon_{10} = \varepsilon_{12} = -1$ and that gives

$$H = Q_4 \oplus Q_4 \oplus -Q_4 \oplus Q_3 \oplus Q_3 \oplus Q_3 \oplus -Q_3 \oplus -Q_3 \oplus Q_3 \oplus -Q_3 \oplus Q_2 \oplus -Q_2.$$

Furthermore, we can see that for the first four choices of η_1, η_2 and η_3, H consists of two positive Q_4 blocks, four positive Q_3 blocks and one positive Q_2 block. For the last four choices of η_1, η_2, η_3, H consists of one positive Q_4 block, three positive Q_3 blocks and one positive Q_2 block.

Thus for the chosen ordering (2.12), the H-selfadjoint matrix B will have an H-selfadjoint fourth root only if the total number of positive Q_4 blocks in H is one or two, the total number of positive Q_3 blocks in H is three or four, and there is only one positive Q_2 block in H.

If the pair (B, H) was given, and therefore ε_j is known for all $j = 1, \ldots, 12$ where some permutations are allowed, Table 2.1 then gives all possible sets of signs η_j for H_A such that (A, H_A) is the canonical form for any H-selfadjoint fourth root of B, associated with the ordering (2.12), if it exists. For example if $\varepsilon_j = 1$ for all $j = 1, \ldots, 12$, then no set of signs η_j for H_A exist, that is, there does not exist an H-selfadjoint fourth root of B associated with this ordering.

We also illustrate the use of (2.3) in this example for the ordering (2.12):

$$\mathcal{B}_\nu^{(k)} = \{i \mid n_i' = \nu;\ 4k-3 \leq i \leq 4k\}$$

where $k = 1, 2, 3$ and $\nu = 4, 3, 2$ (the sizes of the blocks in H). Then $|\mathcal{B}_4^{(1)}| = 3$, $|\mathcal{B}_4^{(2)}| = |\mathcal{B}_4^{(3)}| = 0$, $|\mathcal{B}_3^{(1)}| = 1$, $|\mathcal{B}_3^{(2)}| = 4$, $|\mathcal{B}_3^{(3)}| = 2$, $|\mathcal{B}_2^{(1)}| = |\mathcal{B}_2^{(2)}| = 0$, $|\mathcal{B}_2^{(3)}| = 2$. □

The following example shows how the sign characteristic differs by using different reorderings of the Segre characteristic.

Example 2.2.10. Let $B = \bigoplus_{i=1}^{6} J_3(0) \oplus \bigoplus_{i=1}^{6} J_2(0)$ and be H-selfadjoint where (B, H) is in canonical form. Then the Segre characteristic of B is $3, 3, 3, 3, 3, 3, 2, 2, 2, 2, 2, 2, 0, \ldots$. We illustrate finding the signs of the blocks in H for which an H-selfadjoint sixth root of B exists. For this we consider all of the possible reorderings of the Segre characteristic such that for each 6-tuple, the maximum difference between any two numbers is one. In terms of the notation of Theorem 2.1.3, $n = 30$ and $m = 6$, and in all of the reorderings $p = 2$.

We follow a similar process as the one in Example 2.2.9 to determine the canonical form for (B, H) that is necessary for the existence of an H-selfadjoint sixth root of B for each possible reordering of the Segre characteristic.

1. Reordering: $(3, 3, 3, 3, 3, 3), (2, 2, 2, 2, 2, 2), (0, 0, 0, 0, 0, 0), \ldots$. Canonical form of the H-selfadjoint sixth roots of B: $(J_{18}(0) \oplus J_{12}(0),\ \eta_1 Q_{18} \oplus \eta_2 Q_{12})$. Then

$$\begin{aligned} H = {} & \eta_1 Q_3 \oplus \eta_1 Q_3 \oplus \eta_1 Q_3 \oplus -\eta_1 Q_3 \oplus -\eta_1 Q_3 \oplus -\eta_1 Q_3 \\ & \oplus \eta_2 Q_2 \oplus \eta_2 Q_2 \oplus \eta_2 Q_2 \oplus -\eta_2 Q_2 \oplus -\eta_2 Q_2 \oplus -\eta_2 Q_2. \end{aligned}$$

Thus, for any choice of η_1 and η_2, the number of positive Q_3 blocks in H and the number of positive Q_2 blocks in H are both three.

2. Reordering: $(3,3,3,3,3,2),(3,2,2,2,2,2),(0,0,0,0,0,0),\ldots$. Canonical form of the H-selfadjoint sixth roots of B: $(J_{17}(0)\oplus J_{13}(0),\ \eta_1 Q_{17}\oplus\eta_2 Q_{13})$. Then
$$\begin{aligned}H = {}&\eta_1Q_3\oplus\eta_1Q_3\oplus\eta_1Q_3\oplus-\eta_1Q_3\oplus-\eta_1Q_3\oplus\eta_1Q_2\\ &\oplus\eta_2Q_3\oplus\eta_2Q_2\oplus\eta_2Q_2\oplus\eta_2Q_2\oplus-\eta_2Q_2\oplus-\eta_2Q_2.\end{aligned}$$
Thus, for the choice $\eta_1 = 1$ and $\eta_2 = 1$, the number of positive Q_3 blocks in H and the number of positive Q_2 blocks in H are both four. For both the choices $\eta_1 = 1$, $\eta_2 = -1$, and $\eta_1 = -1$, $\eta_2 = 1$, the number of positive Q_3 blocks and the number of positive Q_2 blocks are both three. If both η_1 and η_2 are chosen as -1, then the number of positive Q_3 blocks and the number of positive Q_2 blocks are both two.

3. Reordering: $(3,3,3,3,2,2),(3,3,2,2,2,2),(0,0,0,0,0,0),\ldots$. Canonical form of the H-selfadjoint sixth roots of B: $(J_{16}(0)\oplus J_{14}(0),\ \eta_1Q_{16}\oplus\eta_2Q_{14})$. Then
$$\begin{aligned}H = {}&\eta_1Q_3\oplus\eta_1Q_3\oplus-\eta_1Q_3\oplus-\eta_1Q_3\oplus\eta_1Q_2\oplus-\eta_1Q_2\\ &\oplus\eta_2Q_3\oplus-\eta_2Q_3\oplus\eta_2Q_2\oplus\eta_2Q_2\oplus-\eta_2Q_2\oplus-\eta_2Q_2.\end{aligned}$$
Thus, as with the first reordering, for any choice of η_1 and η_2, the number of positive Q_3 blocks in H and the number of positive Q_2 blocks in H are both three.

4. Reordering: $(3,3,3,2,2,2),(3,3,3,2,2,2),(0,0,0,0,0,0),\ldots$. Canonical form of the H-selfadjoint sixth roots of B: $(J_{15}(0)\oplus J_{15}(0),\ \eta_1Q_{15}\oplus\eta_2Q_{15})$. Then
$$\begin{aligned}H = {}&\eta_1Q_3\oplus\eta_1Q_3\oplus-\eta_1Q_3\oplus\eta_1Q_2\oplus\eta_1Q_2\oplus-\eta_1Q_2\\ &\oplus\eta_2Q_3\oplus\eta_2Q_3\oplus-\eta_2Q_3\oplus\eta_2Q_2\oplus\eta_2Q_2\oplus-\eta_2Q_2.\end{aligned}$$
Again, the total number of positive blocks in H is the same as with the second reordering. Thus, for the choice $\eta_1 = 1$ and $\eta_2 = 1$, the number of positive Q_3 blocks in H and the number of positive Q_2 blocks in H are both four. For both the choices $\eta_1 = 1$, $\eta_2 = -1$, and $\eta_1 = -1$, $\eta_2 = 1$, the number of positive Q_3 blocks and the number of positive Q_2 blocks are both three. If both η_1 and η_2 are chosen as -1, then the number of positive Q_3 blocks and the number of positive Q_2 blocks are both two.

Note that we have covered all of the possibilities for the sixth root A of B as well as for the corresponding matrix H_A. Therefore this example shows the only options of matrices H that we can start with in canonical form (B, H) from which we will be able to find H-selfadjoint sixth roots. □

We are now ready to prove the theorem giving the conditions of the existence of an H-selfadjoint mth root of nilpotent matrices.

Proof of Theorem 2.2.5. Let B be a nilpotent H-selfadjoint matrix with Segre characteristic $n_1, n_2, \ldots, n_r, 0, \ldots$ and assume there exists an H-selfadjoint matrix A such that $A^m = B$. Let A be similar to $\bigoplus_{k=1}^{p} J_{t_k}(0)$ for some t_k, then from Lemma 2.2.6 we have that the Jordan normal form of A^m is equal to
$$J=\bigoplus_{k=1}^{p}\left[\bigoplus_{i=1}^{r_k}J_{a_k+1}(0)\oplus\bigoplus_{i=1}^{m-r_k}J_{a_k}(0)\right], \tag{2.14}$$

where $t_k = a_k m + r_k$, $a_k, r_k \in \mathbb{Z}$ and $0 < r_k \leq m$ by using the division algorithm. Since $A^m = B$, this matrix J is also the Jordan normal form of B and therefore will have the same Segre characteristic as B, possibly reordered. From (2.14) one can see that this reordering, say $n'_1, n'_2, \ldots, n'_{pm}, 0, \ldots$, has the property that in each m-tuple the difference between the highest and the lowest number is at most one.

From Theorem 2.1.1 the pair $(\bigoplus_{k=1}^p J_{t_k}(0), \bigoplus_{k=1}^p \eta_k Q_{t_k})$ is in canonical form for $\eta_k = \pm 1$. Let the blocks of H_B in the canonical form (J, H_B) after a permutation of blocks according to the reordering $n'_1, n'_2, \ldots, n'_{pm}, 0, \ldots$, be given by $\varepsilon_i Q_{n'_i}$ for $\varepsilon_i = \pm 1$. The conditions on these signs can be found by a change in Jordan basis. The Jordan chains of A^m which correspond to different Jordan blocks of A, or equivalently, to different m-tuples in the above reordering, are considered separately. Among the Jordan chains of A^m of a certain length, say ν, which correspond to a single Jordan block of A, there will be at most one Jordan chain spanning an H-nondegenerate space. This will happen when there is an odd number of Jordan chains of this length since the other Jordan chains of length ν which do not span H-nondegenerate spaces, occur in pairs. By making combinations with these Jordan chains in a similar way as illustrated in Example 2.2.9, we obtain the desired change in Jordan basis. Compare also the proof of Theorem 4.4 in [1]. Each pair of Jordan chains delivers opposite signs of blocks in H_B and the blocks in H_B corresponding to the H-nondegenerate spaces will have the same sign as that obtained from the mth root. Hence by using $\mathcal{B}_\nu^{(k)}$ as introduced in (2.3), we can determine the number of blocks in H_B for each sign. If, for some k, the number $\left|\mathcal{B}_\nu^{(k)}\right|$ is even, then the number of $i \in \mathcal{B}_\nu^{(k)}$ such that $\varepsilon_i = \eta_k$, and the number of $i \in \mathcal{B}_\nu^{(k)}$ such that $\varepsilon_i = -\eta_k$, are both equal to $\frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right|\right)$. If, for some k, the number $\left|\mathcal{B}_\nu^{(k)}\right|$ is odd, then the number of $i \in \mathcal{B}_\nu^{(k)}$ such that $\varepsilon_i = \eta_k$ is $\frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right| + 1\right)$, and the number of $i \in \mathcal{B}_\nu^{(k)}$ such that $\varepsilon_i = -\eta_k$ is $\frac{1}{2}\left(\left|\mathcal{B}_\nu^{(k)}\right| - 1\right)$. Hence, the number of positive blocks in H_B of size ν is equal to

$$\sum_{k=1}^{p} \pi_{\nu,k},$$

where $\pi_{\nu,k}$ is given by (2.8).

Conversely, suppose that (B, H) is in canonical form and that it satisfies Properties 1 and 2, and suppose the reordering of the Segre characteristic of matrix B that satisfies the second property, is given by $n'_1, n'_2, \ldots, n'_{pm}, 0, \ldots$. Let $\tilde{A} = \bigoplus_{k=1}^p J_{t_k}(0)$ where $t_k = \sum_{i=1}^m n'_{m(k-1)+i}$. If we have by the division algorithm that $t_k = a_k m + r_k$, $a_k, r_k \in \mathbb{Z}$, $0 < r_k \leq m$, then from Lemma 2.2.6 the matrix $\tilde{A}^m = \bigoplus_{k=1}^p (J_{t_k}(0))^m$ has the Jordan normal form

$$\bigoplus_{k=1}^{p} \left[\bigoplus_{i=1}^{r_k} J_{a_k+1}(0) \oplus \bigoplus_{i=1}^{m-r_k} J_{a_k}(0) \right].$$

Thus the Segre characteristic of this matrix is some reordering of the numbers in the following m-tuples, with possibly some zeros added:

$$(a_1+1, \ldots, a_1+1, a_1 \ldots, a_1), \ldots, (a_p+1, \ldots, a_p+1, a_p, \ldots, a_p), 0 \ldots. \tag{2.15}$$

Since for all $k = 1, \dots, p$ we have that

$$\sum_{i=1}^{r_k}(a_k+1) + \sum_{i=1}^{m-r_k} a_k = t_k = \sum_{i=1}^{m} n'_{m(k-1)+i} \quad \text{and} \quad n'_{m(k-1)+1} - n'_{mk} \leq 1,$$

it then follows that the Segre characteristic in (2.15) is equal to the sequence

$$n'_1, n'_2, \dots, n'_{pm}, 0, \dots .$$

This means that B is also the Jordan normal form of $\tilde{A}^m$ since they have the same Segre characteristic, or reordering thereof. Note also that the matrix $\tilde{A}$ is H_A-selfadjoint where $H_A = \bigoplus_{k=1}^{p} \varepsilon_k Q_{t_k}$. If we let $\varepsilon_k = \eta_k$ for each k from Property 2 which was assumed for (B, H), then there exists an invertible matrix P, formed in the same way as explained above, such that $P^{-1}\tilde{A}^m P = B$ and $P^* H_A P = H$. Therefore, by Lemma 2.2.1, the matrix $A := P^{-1}\tilde{A}P$ is an H-selfadjoint mth root of B. □

2.2.4 The case where B has only negative eigenvalues

We now look at the case where the eigenvalues of B are negative real numbers, firstly for the case where m is even and secondly where m is odd.

Consider the following example regarding negative eigenvalues.

Example 2.2.11. Let $H = \varepsilon Q_2$, where $\varepsilon = \pm 1$. Suppose that the H-selfadjoint matrix

$$B = J_2(-1) = \begin{bmatrix} -1 & 1 \\ 0 & -1 \end{bmatrix}$$

has a square root A which is H-selfadjoint. We know that $\sigma(A) \subseteq \{i, -i\}$ since i and $-i$ are the square roots of -1. According to Theorem 2.1.1 the Jordan normal form of A should be

$$J = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix},$$

which is Q_2-selfadjoint. Let $A = S^{-1}JS$ for an invertible matrix S, then

$$A^2 = (S^{-1}JS)^2 = S^{-1}\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} S,$$

which is not similar to B. This gives a contradiction. Therefore, B does not have a square root which is H-selfadjoint. Note however, that $\begin{bmatrix} i & -\frac{1}{2}i \\ 0 & i \end{bmatrix}^2 = B$, so B does in fact have a square root. □

This illustrates the fact that there do not exist H-selfadjoint mth roots of matrices of the form $J_n(\lambda)$ where m is even and λ is a negative real number. Suppose in general that $B = J_n(\lambda)$, with λ a negative real eigenvalue. We know from Theorem 2.1.1 that $(B, \varepsilon Q_n)$ is in canonical form. But the mth roots of λ, where m is even, are all nonreal numbers, since no real number raised to the mth power can be negative if m is even. Therefore the eigenvalues of any mth root A of B are nonreal numbers. From Theorem 2.1.1 we know that the Jordan normal form of A should contain pairs of Jordan blocks of equal size that correspond to complex conjugate pairs. This implies that the Jordan normal form of A should consist of a direct sum of at least two blocks of equal size, but such a matrix raised to the mth power is not similar to B. Hence, the blocks of the canonical form of (B, H) corresponding to negative real eigenvalues should occur in pairs.

Now we present a lemma that will be useful in the proof of the subsequent theorem.

Lemma 2.2.12. *Let T be an upper triangular complex $n \times n$ Toeplitz matrix with $\lambda \in \mathbb{R}$ on the main diagonal, and a nonzero number on the first superdiagonal. Let $B = T \oplus \overline{T}$. Then B is Q_{2n}-selfadjoint, and the pair (B, Q_{2n}) is unitarily similar to $(J_n(\lambda) \oplus J_n(\lambda), Q_n \oplus -Q_n)$.*

Proof. Let

$$T = \begin{bmatrix} \lambda & t_2 & \cdots & t_n \\ & \ddots & \ddots & \vdots \\ & & \ddots & t_2 \\ & & & \lambda \end{bmatrix},$$

with $t_2 \neq 0$. Then

$$Q_{2n}B = \begin{bmatrix} 0 & Q_n \\ Q_n & 0 \end{bmatrix} \begin{bmatrix} T & 0 \\ 0 & \overline{T} \end{bmatrix} = \begin{bmatrix} 0 & Q_n\overline{T} \\ Q_n T & 0 \end{bmatrix}$$

$$= \begin{bmatrix} & & & & & & & \lambda \\ & & & & & & \iddots & \overline{t_2} \\ & & & & & \iddots & \iddots & \vdots \\ & & & & \lambda & \overline{t_2} & \cdots & \overline{t_n} \\ & & & \lambda & & & & \\ & & \iddots & t_2 & & & & \\ & \iddots & \iddots & \vdots & & & & \\ \lambda & t_2 & \cdots & t_n & & & & \end{bmatrix}$$

which is clearly selfadjoint. Hence, B is Q_{2n}-selfadjoint.

Because $t_1 = \lambda$ is real and $t_2 \neq 0$, the Jordan normal form of both T and $\overline{T}$ is $J_n(\lambda)$. Thus the canonical form of the pair (B, Q_{2n}) is given by $(J_n(\lambda) \oplus J_n(\lambda), \varepsilon_1 Q_n \oplus \varepsilon_2 Q_n)$. Therefore, there exists an invertible matrix S such that $S^{-1}BS = J_n(\lambda) \oplus J_n(\lambda)$ and $S^* Q_{2n} S = \varepsilon_1 Q_n \oplus \varepsilon_2 Q_n$. By using these equations and letting $Q = \varepsilon_1 Q_n \oplus \varepsilon_2 Q_n$, we have the following congruence:

$$S^* Q_{2n} BS = S^* Q_{2n} S S^{-1} BS = Q\,(J_n(\lambda) \oplus J_n(\lambda)),$$

which leads to

$$S^* Q_{2n}(B - \lambda I)S = Q\,(J_n(0) \oplus J_n(0)),$$

and then by multiplying $(S^{-1}(B - \lambda I)S)^{n-2}$ from the right, we have

$$S^* Q_{2n}(B - \lambda I)^{n-1} S = Q\,(J_n(0) \oplus J_n(0))^{n-1}. \tag{2.16}$$

Note that the matrix $Q_{2n}(B-\lambda I)^{n-1}$ has only two nonzero entries: t_2^{n-1} in the $(2n,n)$ position and its complex conjugate in the $(n,2n)$ position. Consequently, $Q_{2n}(B-\lambda I)^{n-1}$ has only one positive and one negative eigenvalue, namely $\pm(t_2\overline{t_2})^{\frac{n-1}{2}}$, and the matrix on the right side of (2.16) has eigenvalues ε_1 and ε_2. Hence, by Sylvester's law of inertia $\varepsilon_1=-\varepsilon_2$, and by reordering the Jordan blocks if necessary, we have that the pair (B,Q_{2n}) is unitarily similar to $(J_n(\lambda)\oplus J_n(\lambda), Q_n\oplus -Q_n)$ as claimed. □

First we consider the case where m is even.

Theorem 2.2.13. *Let B be an H-selfadjoint matrix with a spectrum consisting of only negative real numbers. Then there exists an H-selfadjoint matrix A such that $A^m=B$, for m even, if and only if the canonical form of (B,H), given by (J,H_B), has the following form:*

$$J=\bigoplus_{j=1}^{t}\left(J_{k_j}(\lambda_j)\oplus J_{k_j}(\lambda_j)\right),\quad \lambda_j\in\mathbb{R}^- \tag{2.17}$$

and

$$H_B=\bigoplus_{j=1}^{t}\left(Q_{k_j}\oplus(-Q_{k_j})\right). \tag{2.18}$$

Proof. Let B be an H-selfadjoint matrix with a spectrum consisting of only negative real numbers and assume there exists an H-selfadjoint matrix A such that $A^m=B$, with m even. Then the eigenvalues of A, which are mth roots of negative real numbers $\lambda_j\in\sigma(B)$, will be nonreal numbers. Since A is H-selfadjoint, the eigenvalues of A must be symmetric relative to the real axis. Therefore, by Theorem 2.1.1, the canonical form of (A,H) is of the form

$$\left(\bigoplus_{j=1}^{t}\left(J_{k_j}(\mu_j)\oplus J_{k_j}(\bar{\mu}_j)\right),\ \bigoplus_{j=1}^{t}Q_{2k_j}\right),$$

where μ_j is an mth root of $\lambda_j\in\mathbb{R}^-$. This means that there exists an invertible matrix S such that

$$S^{-1}AS=\bigoplus_{j=1}^{t}\left(J_{k_j}(\mu_j)\oplus J_{k_j}(\bar{\mu}_j)\right)\quad\text{and}\quad S^*HS=\bigoplus_{j=1}^{t}Q_{2k_j}.$$

Consider $S^{-1}BS=(S^{-1}AS)^m=\bigoplus_{j=1}^{t}\left(\left(J_{k_j}(\mu_j)\right)^m\oplus\left(J_{k_j}(\bar{\mu}_j)\right)^m\right)$, which is $S^*HS=\bigoplus_{j=1}^{t}Q_{2k_j}$-selfadjoint. By Lemma 2.2.12, it follows that the canonical form of (B,H) is

$$\left(\bigoplus_{j=1}^{t}\left(J_{k_j}(\lambda_j)\oplus J_{k_j}(\lambda_j)\right),\ \bigoplus_{j=1}^{t}\left(Q_{k_j}\oplus(-Q_{k_j})\right)\right).$$

Conversely, let B be an H-selfadjoint matrix and assume that the canonical form of (B,H) is as in (2.17) and (2.18). We first consider the case of just one pair of blocks, so assume

$$B=J_n(\lambda)\oplus J_n(\lambda)\quad\text{and}\quad H=Q_n\oplus(-Q_n),$$

with λ a negative real number. Let μ be an arbitrary mth root of λ, and let $\tilde{A}=J_n(\mu)\oplus J_n(\bar{\mu})$. Since m is even and $\lambda<0$, we have that μ is nonreal; therefore the matrix $\tilde{A}$ is Q_{2n}-selfadjoint. Now, note that $\tilde{A}^m$ has λ on the main diagonal and then Lemma 2.2.12 implies that the pairs $(\tilde{A}^m, Q_{2n})$ and (B, H) are unitarily similar. Hence, there exists an invertible matrix P such that the equations

$$P^{-1}\tilde{A}^m P = B \text{ and } P^* Q_{2n} P = H$$

hold. From Lemma 2.2.1 the matrix $A := P^{-1}\tilde{A}P$ is an H-selfadjoint mth root of B. In the case where B consists of more than one pair of blocks, the construction can be applied to each pair of blocks separately. □

For the case where m is odd the following result holds.

Theorem 2.2.14. *Let B be an H-selfadjoint matrix with a spectrum consisting only of negative real numbers. Then, for m odd, there exists an H-selfadjoint matrix A such that $A^m = B$.*

Proof. Let B be an $n \times n$ H-selfadjoint matrix with negative real eigenvalues. Assume that the pair (B, H) is in canonical form and that B consists of a single Jordan block, that is,

$$B = J_n(\lambda) \quad \text{and} \quad H = \varepsilon Q_n,$$

where $\varepsilon = \pm 1$ and λ is a negative real number. Let μ be the real mth root of λ, and let $\tilde{A} = J_n(\mu)$. Then the Jordan normal form of $\tilde{A}^m$ is equal to B. Note that the matrix $\tilde{A}$ is H_A-selfadjoint where $H_A = \delta Q_n$, with $\delta = 1$ or $\delta = -1$. Take $\delta = \varepsilon$. Similarly as in Section 2.2.1, construct an invertible matrix P such that the equations

$$P^{-1}\tilde{A}^m P = B \text{ and } P^* H_A P = H$$

hold. Finally, it follows from Lemma 2.2.1 that the matrix $A := P^{-1}\tilde{A}P$ is an H-selfadjoint mth root of B. In the case where B consists of more than one block, the construction is applied to each block separately. □

We illustrate Theorem 2.2.14 with the following example.

Example 2.2.15. Let $m = 5$ and let the matrices B and H be given by

$$B = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \quad \text{and} \quad H = Q_3 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

Then (B, H) is in canonical form. The eigenvalues of any fifth root of the matrix B are fifth roots of -1. Construct the following matrix by using the real fifth root of -1, that is, let $\tilde{A} = J_3(-1)$. Note that $\tilde{A}$ is H_A-selfadjoint, where $H_A = Q_3$. Then

$$\tilde{A}^5 = \begin{bmatrix} -1 & 5 & -10 \\ 0 & -1 & 5 \\ 0 & 0 & -1 \end{bmatrix}.$$

Using the notation in Section 2.2.1, one can easily see that

$$p_1 = \begin{bmatrix} 25y_3 \\ 0 \\ 0 \end{bmatrix}, \ p_2 = \begin{bmatrix} 5y_2 - 10y_3 \\ 5y_3 \\ 0 \end{bmatrix} \text{ and } p_3 = y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix},$$

so we obtain the equations:

$$1 = \phi_1(y) = y^* H_A(\tilde{A}^5 + I)^2 y = 25\bar{y}_3 y_3,$$

$$0 = \phi_2(y) = y^* H_A(\tilde{A}^5 + I) y = 5\bar{y}_3 y_2 - 10\bar{y}_3 y_3 + 5\bar{y}_2 y_3,$$
$$0 = \phi_3(y) = y^* H_A y = \bar{y}_3 y_1 + \bar{y}_2 y_2 + \bar{y}_1 y_3.$$

One solution of these equations is the real vector y where $y_3 = 1/5$, $y_2 = 1/5$ and $y_1 = -1/10$. Thus we have a matrix

$$P = \begin{bmatrix} 5 & -1 & \frac{-1}{10} \\ 0 & 1 & \frac{1}{5} \\ 0 & 0 & \frac{1}{5} \end{bmatrix},$$

such that the equations $P^{-1}\tilde{A}^5 P = B$ and $P^* H_A P = H$ hold. Finally, we note that the matrix

$$A = P^{-1}\tilde{A}P = \begin{bmatrix} -1 & \frac{1}{5} & \frac{2}{25} \\ 0 & -1 & \frac{1}{5} \\ 0 & 0 & -1 \end{bmatrix}$$

is an H-selfadjoint fifth root of B. □

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Chapter 3

Complex H-nonnegative square roots[1]

Abstract. Roots of matrices are well-studied. The conditions for their existence are understood: The block sizes of nilpotent Jordan blocks, arranged in pairs, have to satisfy some simple algebraic property.

More interesting are structured roots of structured matrices. Probably the best known example is the existence and uniqueness of positive definite square roots of a positive definite matrix. If one drops the requirement of positive definiteness of the square root, it turns out that there exists an abundance of square roots. Here a description of all canonical forms of all square roots is possible and is straight forward.

H-nonnegative matrices are H-selfadjoint and are nonnegative with respect to an indefinite inner product with an invertible Hermitian matrix H. An H-nonnegative matrix B allows a decomposition in a negative definite, a nilpotent H-nonnegative, and a positive definite matrix, $B = B_- \oplus B_0 \oplus B_+$. The interesting part is B_0, as only Jordan blocks of size one and two occur. Determining a square root of B reduces to determining a square root of each of B_-, B_0, and B_+. Here we investigate for an H-nonnegative matrix its square roots without additional structure, as well as its structured square roots that are H-nonnegative or H-selfadjoint.

For these three classes of square roots of H-nonnegative matrices we show a simple criterion for their existence and describe all possible canonical forms. This is based mainly on known results, but an important new part is that in all three cases we describe all possible square roots of the nilpotent H-nonnegative matrix B_0 explicitly. Moreover, we show how our results can be applied to the conditional and unconditional stability of H-nonnegative square roots of H-nonnegative matrices, where the explicit description of the square roots of B_0 is used.

Keywords. Indefinite inner products, Square roots, H-nonnegative matrices.
AMS subject classifications. 15A21, 15A23, 47B50.

3.1 Introduction

The study of square roots of matrices dates back to 1858 [8]. Since 1858 numerous authors have studied square roots of matrices. For example, a necessary and sufficient condition for the existence of square roots of a complex matrix A is given in [9]. This condition relates

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to the dimensions of nullspaces of powers of A. Other authors such as [2, 10, 14, 15, 17], to mention but a few, focus on an efficient algorithm or a formula for square roots of a matrix.

The problem of finding roots of matrices where certain extra requirements or structure are imposed on the class of matrices studied and/or their roots, has also attracted a lot of attention. For example, [1] studies roots of M-matrices that are M-matrices themselves and [11] find results on Hamiltonian square roots of skew-Hamiltonian matrices.

Turning to indefinite inner product spaces, by definition $[x, y] = \langle Hx, y\rangle$ represents the indefinite inner product between vectors x and y in $\mathbb{C}^n$ where H is some Hermitian and invertible matrix. Here $\langle\cdot\,,\cdot\rangle$ is the standard inner product in $\mathbb{C}^n$. A complex $n \times n$ matrix B is called *H-selfadjoint* if $[Bx, y] = [x, By]$, that is, if $HB = B^*H$. In [4] and [16] H-selfadjoint square roots of H-selfadjoint matrices are studied. The canonical form of all H-selfadjoint matrices having H-selfadjoint square roots is derived, as well as the canonical form of the H-selfadjoint square roots.

A complex matrix B is called *H-nonnegative* if $[Bx, x] \geq 0$ for all $x \in \mathbb{C}^n$. The class of H-nonnegative matrices is a subclass of the class of H-selfadjoint matrices and has some very special properties, such as having a real spectrum and having Jordan blocks of size at most two. We study square roots of H-nonnegative matrices and in Section 3.3 we find necessary and sufficient conditions for the existence of square roots. We also give explicit formulas for the square roots of nilpotent matrices. In Section 3.4 we characterize all H-selfadjoint square roots of H-nonnegative matrices and find characterizations of an H-nonnegative matrix with entries in $\mathbb{C}$ to have H-selfadjoint square roots, while in Section 3.5 we find conditions for an H-nonnegative matrix to have an H-nonnegative square root. Finally, Section 3.6 contains the theory regarding the stability of these H-nonnegative square roots.

3.2 Preliminaries

The Jordan normal form plays an important role in this chapter. We denote an $n \times n$ Jordan block corresponding to an eigenvalue λ in a Jordan normal form by $J_n(\lambda)$ and the $n \times n$ sip matrix which has ones on the main anti-diagonal and zeros elsewhere by Q_n. Here "sip" stands for standard involutory permutation.

Let B be a square matrix which at eigenvalue λ has in its Jordan normal form Jordan blocks of sizes in decreasing order $(n_1, n_2, n_3, \ldots, n_r)$. We call this the *Segre characteristic*[2] of matrix B corresponding to the eigenvalue λ (see for example the book by Shapiro [18]).

In the following theorem we recall the well-known canonical form given by (3.1) and (3.2) for a pair (B, H), where B is an H-selfadjoint matrix and H is an invertible Hermitian matrix (see for example [13]).

Theorem 3.2.1. *Let H be an invertible Hermitian $n \times n$ matrix, and let B be an $n \times n$ complex H-selfadjoint matrix. Then there exists an invertible $n \times n$ matrix S such that*

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[2] Here the Segre characteristic is defined somewhat differently than in Chapters 2 and 4, but the difference is cosmetic and entails zeros that are dropped. In our subsequent definition of a Segre pairing we do consider the zeros again.

$S^{-1}BS$ and S^*HS have the form

$$\begin{aligned} S^{-1}BS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus \ [J_{k_{\alpha+1}}(\lambda_{\alpha+1}) \oplus J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1})] \oplus \cdots \oplus [J_{k_\beta}(\lambda_\beta) \oplus J_{k_\beta}(\overline{\lambda}_\beta)] \end{aligned} \tag{3.1}$$

where $\lambda_1, \ldots, \lambda_\alpha$ are real and $\lambda_{\alpha+1}, \ldots, \lambda_\beta$ are nonreal with positive imaginary parts; and

$$S^*HS = \varepsilon_1 Q_{k_1} \oplus \cdots \oplus \varepsilon_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta} \tag{3.2}$$

where $\varepsilon_1, \ldots, \varepsilon_\alpha$ are ± 1. For a given pair (B, H), the canonical form given by (3.1) and (3.2) is unique up to permutation of orthogonal components in (3.2) and the same simultaneous permutation of the corresponding blocks in (3.1).

Observe that only the blocks in (3.2) related to blocks in (3.1) with a real eigenvalue possess a sign. The vector of signs $(\varepsilon_1, \ldots, \varepsilon_\alpha)$ is called the *sign characteristic* of (B, H).

In the canonical form given by (3.1) and (3.2), for any $i = 1, \ldots, \alpha$, we say the block $J_{k_i}(\lambda_i)$ has *positive sign characteristic* if $\varepsilon_i = 1$, and *negative sign characteristic* if $\varepsilon_i = -1$.

H-nonnegative matrices have the following characteristics (taken from [13, Theorem 5.7.2]).

Theorem 3.2.2. *A matrix B is H-nonnegative if and only if the following conditions hold:*

(i) *B is H-selfadjoint;*

(ii) *B has a real spectrum;*

(iii) *the canonical form of the pair (B, H) is:*

$$S^{-1}BS = \bigoplus_{i=1}^{q} J_1(\lambda_i) \oplus \bigoplus_{i=1}^{r-q} J_1(\lambda_{q+i}) \oplus \bigoplus_{i=1}^{s} J_1(0) \oplus \bigoplus_{i=1}^{t} J_2(0),$$

$$S^*HS = \bigoplus_{i=1}^{q} Q_1 \oplus \bigoplus_{i=1}^{r-q} (-Q_1) \oplus \bigoplus_{i=1}^{s} \varepsilon_i Q_1 \oplus \bigoplus_{i=1}^{t} Q_2,$$

where $\lambda_1, \ldots, \lambda_q > 0$, $\lambda_{q+1}, \ldots, \lambda_r < 0$, and $\varepsilon_i = \pm 1$. Thus B has positive sign characteristic at a nonzero eigenvalue λ if $\lambda > 0$, and negative sign characteristic if $\lambda < 0$; each Jordan block of size 2 at the zero eigenvalue has positive sign characteristic.

We frequently require Theorem 3.1 from [16] in some of the sections and therefore present it here in an equivalent form without the "moreover" part.

Theorem 3.2.3. *Let B be an H-selfadjoint matrix. Then there exists an H-selfadjoint matrix A such that $A^2 = B$ if and only if the canonical form of (B, H) has the following properties:*

(i) *the Jordan blocks corresponding to the negative eigenvalues exist in pairs and the two Jordan blocks in each pair have opposite sign characteristic;*

(ii) *the Jordan blocks corresponding to the zero eigenvalue can be written as* $J^{(1)} \oplus J^{(2)} \oplus J^{(3)}$*, where* $J^{(1)}$ *is a direct sum of pairs* $J_{p_i}(0) \oplus J_{p_i}(0)$*,* $J^{(2)}$ *is a direct sum of pairs* $J_{p_i}(0) \oplus J_{p_i-1}(0)$ *and* $J^{(3)}$ *is a direct sum of* 1×1 *blocks and where the blocks in each pair in* $J^{(1)}$ *have opposite sign characteristic and those in each pair in* $J^{(2)}$ *have the same sign characteristic.*

3.3 Square roots

In this section we describe all square roots of H-nonnegative matrices, that is, the collection of all matrices A such that $A^2 = B$ and B is H-nonnegative. Without loss of generality we always assume B to be in Jordan normal form. The following result is well-known (see for example [7]).

Theorem 3.3.1. *Let* B *be* H*-nonnegative and in Jordan normal form. Write* B *as*

$$B = B_- \oplus B_0 \oplus B_+, \tag{3.3}$$

where $\sigma(B_\pm) \subset \mathbb{R}^\pm$ *and* $\sigma(B_0) = \{0\}$*. A matrix* A *is a square root of* B *if and only if there exist square roots* A_-*,* A_0*, and* A_+ *of* B_-*,* B_0*, and* B_+*, respectively, such that*

$$A = A_- \oplus A_0 \oplus A_+. \tag{3.4}$$

Proof. The partition of B follows from Theorem 3.2.2. Given square roots A_-, A_0, and A_+ of B_-, B_0, and B_+, respectively, it is obvious that $A_- \oplus A_0 \oplus A_+$ is a square root of B. We show the converse. Let A be a square root of B, that is, $A^2 = B$. Therefore, A and B commute and, by [12, Theorem 3 in Chapter VIII], A allows a representation as in (3.4). As $A^2 = A_-^2 \oplus A_0^2 \oplus A_+^2$ we conclude that A_-, A_0, and A_+ are square roots of B_-, B_0, and B_+, respectively. ☐

It follows from Theorem 3.2.2 that B_- and B_+ are diagonalizable and, hence, they have a square root. Therefore a square root of B exists if and only if a square root of B_0 exists according to Theorem 3.3.1. For this reason, we focus on the case where $B = B_0$ is a nilpotent H-nonnegative matrix. Let $(n_1, n_2, \ldots, n_r)$ be the Segre characteristic of B_0. We call a collection $\mathcal{S}$ of pairs of numbers from $\mathcal{N} = \{n_i\}_{i=1}^r \cup \{0\}$ a *Segre pairing* if:

- each entry in the Segre characteristic appears in one and only one pair of $\mathcal{S}$;
- each pair in $\mathcal{S}$ consists of two entries from the Segre characteristic or one entry from the Segre characteristic and one zero, with the first entry greater or equal to the second entry;
- the absolute difference between the two entries in each pair is at most one;
- the pairs are arranged lexicographically.

Note that a pair of the form $(4, 2)$, $(2, 0)$ or $(0, 0)$ is not a member of a Segre pairing. In [7] it is shown that a matrix B_0 has a square root if and only if there exists a Segre pairing. By Theorem 3.2.2 we know that for each pair (m, n) in a Segre pairing of an H-nonnegative matrix B_0, we have $m \leq 2$, $n \leq 2$ and $|m - n| \leq 1$. This leads to the following characterization of square roots of a nilpotent H-nonnegative matrix.

Theorem 3.3.2. *Let B_0 be a nilpotent H-nonnegative matrix. Then the following are equivalent:*

(i) *B_0 has a square root;*

(ii) *There exists a Segre pairing;*

(iii) *In the Segre characteristic of B_0, either there is an even number of entries equal to two, or there is an odd number of entries equal to two and at least one entry equal to one.*

Proof. The items (i) and (ii) are equivalent, see [7].

By the definition of Segre pairing, assertion (ii) implies assertion (iii).

For the proof that (iii) implies (ii), we pair all the entries in the Segre characteristic equal to two. If there is an odd number of entries equal to two, pair one 2 in the Segre characteristic with a 1. Pair the rest of the entries equal to one with other entries equal to one or with a zero. This forms a Segre pairing. □

In the following theorem we describe all square roots of a nilpotent H-nonnegative matrix related to a pair in $\mathcal{S}$, which can be made explicit. As a by-product we also obtain the Jordan normal form.

Theorem 3.3.3. *Let B_0 be a nilpotent H-nonnegative matrix in Jordan normal form which has a Segre pairing $\mathcal{S}$. Any pair of $\mathcal{S}$ is of the form*

$$(2,2),\ (2,1),\ (1,1)\ \textit{or}\ (1,0). \tag{3.5}$$

These pairs correspond to Jordan blocks of the form $J_2(0)\oplus J_2(0)$, $J_2(0)\oplus J_1(0)$, $J_1(0)\oplus J_1(0)$ and $J_1(0)$, respectively, in the matrix B_0. The square roots of each possible pair in $\mathcal{S}$ are as follows:

(i) *The square root of $J_1(0) = [0]$, which is associated with the pair $(1,0)$, is equal to $[0]$. Its Jordan normal form is $J_1(0)$ again.*

(ii) *The square roots of $J_1(0) \oplus J_1(0)$, which is associated with the pair $(1,1)$, are either of the form*

$$\begin{bmatrix} \alpha & \frac{-\alpha^2}{\beta} \\ \beta & -\alpha \end{bmatrix},\ \textit{for any complex numbers } \alpha, \beta \textit{ with } \beta \neq 0, \tag{3.6}$$

$$\textit{or}\ \begin{bmatrix} 0 & \alpha \\ 0 & 0 \end{bmatrix},\ \textit{for any complex number } \alpha. \tag{3.7}$$

The Jordan normal form of all matrices in (3.6) and (3.7) is $J_2(0)$, except in the case in (3.7) where $\alpha = 0$. In this case, the Jordan normal form is $J_1(0) \oplus J_1(0)$.

(iii) *The square roots of $J_2(0) \oplus J_1(0)$, which is associated with the pair $(2,1)$, are of the form*

$$\begin{bmatrix} 0 & \alpha & \beta \\ 0 & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \end{bmatrix},\ \textit{for complex numbers } \alpha \textit{ and } \beta \neq 0. \tag{3.8}$$

The Jordan normal form of all matrices in (3.8) is $J_3(0)$.

(iv) *The square roots of* $J_2(0) \oplus J_2(0)$*, which is associated with the pair* $(2,2)$*, are either of the form*

$$\begin{bmatrix} -\gamma_3 & -\gamma_4 & \frac{-\gamma_3^2}{\gamma_1} & \alpha_4 \\ 0 & -\gamma_3 & 0 & \frac{-\gamma_3^2}{\gamma_1} \\ \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\ 0 & \gamma_1 & 0 & \gamma_3 \end{bmatrix}, \tag{3.9}$$

for complex numbers γ_i*, a nonzero* γ_1*, and where* $\alpha_4 = \frac{1}{\gamma_1^2}(\gamma_1 + \gamma_3^2\gamma_2 - 2\gamma_1\gamma_3\gamma_4)$*, or*

$$\begin{bmatrix} 0 & \gamma_1 & \gamma_2 & \gamma_3 \\ 0 & 0 & 0 & \gamma_2 \\ 0 & \frac{1}{\gamma_2} & 0 & -\gamma_1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{3.10}$$

for complex numbers γ_i*, and nonzero* γ_2*. The Jordan normal form of all matrices in* (3.9) *and* (3.10) *is* $J_4(0)$*.*

Proof. The first statement follows from the form of B_0 according to Theorem 3.2.2. It can easily be checked that each of the matrices described in items (i) to (iv) is indeed a square root of the given matrix. The necessity of the forms follows now per item.

Part (i) is trivial since the square root of a 1×1 zero matrix is the 1×1 zero matrix.

Part (ii): Consider a nilpotent matrix in Jordan normal form with Segre characteristic $(1,1)$, i.e. the 2×2 zero matrix. Let A be a square root, that is, $A^2 = \left[\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right]$. Then for the two unit vectors e_1, e_2 in $\mathbb{C}^2$ we have $A^2 e_1 = 0$ and $A^2 e_2 = 0$. Let

$$\begin{aligned} Ae_1 &= \alpha_1 e_1 + \beta_1 e_2, \\ Ae_2 &= \alpha_2 e_1 + \beta_2 e_2, \end{aligned} \tag{3.11}$$

where the coefficients α_j and β_j are complex numbers. Multiply these equations by A and use them again. Then we obtain the equations:

$$\begin{aligned} \alpha_1^2 + \alpha_2\beta_1 &= 0, \\ \beta_2^2 + \alpha_2\beta_1 &= 0, \\ \beta_1(\alpha_1 + \beta_2) &= 0, \\ \alpha_2(\alpha_1 + \beta_2) &= 0. \end{aligned}$$

Assume that β_1 is nonzero, then $\alpha_1 = -\beta_2$ and $\alpha_2 = -\beta_2^2/\beta_1$. This gives the form of any square root, with left-lower entry nonzero, of the zero matrix of size 2×2:

$$\begin{bmatrix} -\beta_2 & \frac{-\beta_2^2}{\beta_1} \\ \beta_1 & \beta_2 \end{bmatrix},$$

which shows (3.6). Moreover, (3.11) implies $Ae_1 \neq 0$. As $A^2 e_1 = 0$ we see that the Jordan normal form of the matrix in (3.6) is $J_2(0)$. Note that if $\beta_1 = 0$, then $\alpha_1 = \beta_2 = 0$, and the square root is

$$\begin{bmatrix} 0 & \alpha_2 \\ 0 & 0 \end{bmatrix},$$

for any complex number α_2.

Part (iii): Consider a nilpotent matrix in Jordan normal form with Segre characteristic $(2, 1)$:

$$J_2(0) \oplus J_1(0) = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and let A be a square root such that $A^2 = J_2(0) \oplus J_1(0)$. Let e_1, e_2, e_3 denote the three unit vectors in $\mathbb{C}^3$. We have

$$A^2 e_1 = 0; \quad A^2 e_2 = e_1; \quad A^2 e_3 = 0. \tag{3.12}$$

Let

$$Ae_j = \alpha_j e_1 + \beta_j e_2 + \gamma_j e_3, \tag{3.13}$$

for $j = 1, 2, 3$, where $\alpha_j, \beta_j, \gamma_j$ are complex numbers. Multiply every equation in (3.12) by the matrix A and compare with the equations in (3.13) multiplied by A^2, then

$$\beta_1 e_1 = 0; \quad \beta_3 e_1 = 0; \quad \beta_2 e_1 = Ae_1. \tag{3.14}$$

From the first two equations it follows that $\beta_1 = 0$, $\beta_3 = 0$, and from the last equation in (3.14) using (3.13) with $j = 1$ we get

$$\beta_2 e_1 = \alpha_1 e_1 + \gamma_1 e_3,$$

which gives $\gamma_1 = 0$ and $\beta_2 = \alpha_1$. Also, we multiply the last equation in (3.14) by A and use (3.12) to get $\beta_2 = 0$ and consequently $\alpha_1 = 0$. Hence $Ae_1 = 0$. Next, we take the expressions for Ae_2 and Ae_3 in (3.13), multiply both sides by A, and use the equations in (3.13), (3.12) and $Ae_1 = 0$ to obtain

$$\begin{aligned} 0 = A^2 e_3 = \gamma_3 A e_3 &= \gamma_3 \alpha_3 e_1 + \gamma_3^2 e_3, \\ e_1 = A^2 e_2 = \gamma_2 A e_3 &= \gamma_2 \alpha_3 e_1 + \gamma_2 \gamma_3 e_3. \end{aligned}$$

From the first equation we conclude that $\gamma_3 = 0$ and then it follows from the second equation that $\gamma_2 \alpha_3 = 1$. Thus any square root of the matrix $J_2(0) \oplus J_1(0)$ is given by:

$$\begin{bmatrix} 0 & \alpha_2 & \alpha_3 \\ 0 & 0 & 0 \\ 0 & \gamma_2 & 0 \end{bmatrix}, \tag{3.15}$$

where $\alpha_2, \alpha_3, \gamma_2$ are any complex numbers such that $\gamma_2 \alpha_3 = 1$. Then

$$Ae_2 = \alpha_2 e_1 + \gamma_2 e_3, \quad A(\alpha_2 e_1 + \gamma_2 e_3) = \gamma_2 \alpha_3 e_1 = e_1, \quad Ae_1 = 0,$$

and from $\gamma_2 \alpha_3 = 1$, it follows that (3.15) has Jordan normal form $J_3(0)$.

Part (iv): Consider a nilpotent matrix in Jordan normal form with Segre characteristic $(2, 2)$:

$$J_2(0) \oplus J_2(0) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

and let A be a square root such that $A^2 = J_2(0) \oplus J_2(0)$. Let $e_1, \dots, e_4$ be the four unit vectors in $\mathbb{C}^4$. Then we have

$$A^2e_1 = 0; \quad A^2e_2 = e_1; \quad A^2e_3 = 0; \quad A^2e_4 = e_3. \tag{3.16}$$

Now, let

$$Ae_j = \alpha_j e_1 + \beta_j e_2 + \gamma_j e_3 + \delta_j e_4, \tag{3.17}$$

for $j = 1, 2, 3, 4$, and where all coefficients are complex numbers. Now we multiply each equation in (3.17) by A^2 and using (3.16) we obtain

$$A^3e_j = \beta_j e_1 + \delta_j e_3, \quad j = 1, \dots, 4. \tag{3.18}$$

By taking $j = 1$ and $j = 3$ in (3.18) and using (3.16) we obtain $\beta_1 = \delta_1 = \beta_3 = \delta_3 = 0$. Using (3.16) again, the equations in (3.18) for $j = 2$ and $j = 4$ become

$$Ae_1 = \beta_2 e_1 + \delta_2 e_3 \quad \text{and} \quad Ae_3 = \beta_4 e_1 + \delta_4 e_3. \tag{3.19}$$

From (3.17) we also have

$$Ae_1 = \alpha_1 e_1 + \gamma_1 e_3, \quad Ae_3 = \alpha_3 e_1 + \gamma_3 e_3, \tag{3.20}$$

and when we compare the coefficients of the unit vectors in (3.19) and (3.20) we obtain the following:

$$\beta_2 = \alpha_1, \ \delta_2 = \gamma_1, \ \beta_4 = \alpha_3, \ \delta_4 = \gamma_3.$$

Then the equations in (3.17) with $j = 2$ and $j = 4$ become

$$\begin{aligned} Ae_2 &= \alpha_2 e_1 + \alpha_1 e_2 + \gamma_2 e_3 + \gamma_1 e_4, \\ Ae_4 &= \alpha_4 e_1 + \alpha_3 e_2 + \gamma_4 e_3 + \gamma_3 e_4. \end{aligned} \tag{3.21}$$

Finally, we multiply the expressions for Ae_1 and Ae_3 in (3.20) by A and use the equations in (3.16), then:

$$\begin{aligned} j = 1: &\quad 0 = \alpha_1 Ae_1 + \gamma_1 Ae_3 = (\alpha_1^2 + \gamma_1\alpha_3)e_1 + (\alpha_1\gamma_1 + \gamma_1\gamma_3)e_3, \\ j = 3: &\quad 0 = \alpha_3 Ae_1 + \gamma_3 Ae_3 = (\alpha_3\alpha_1 + \gamma_3\alpha_3)e_1 + (\alpha_3\gamma_1 + \gamma_3^2)e_3. \end{aligned} \tag{3.22}$$

From this we obtain equalities which gives

$$\alpha_1 = -\gamma_3, \quad \alpha_3 = \frac{-\gamma_3^2}{\gamma_1},$$

where we assume that $\gamma_1 \neq 0$. Using these expressions together with (3.16), and doing the same with Ae_2 from (3.21), we have

$$\begin{aligned} e_1 &= A(\alpha_2 e_1 + \alpha_1 e_2 + \gamma_2 e_3 + \gamma_1 e_4) \\ &= \alpha_2(\alpha_1 e_1 + \gamma_1 e_3) - \gamma_3(\alpha_2 e_1 - \gamma_3 e_2 + \gamma_2 e_3 + \gamma_1 e_4) + \gamma_2(\alpha_3 e_1 + \gamma_3 e_3) \\ &\qquad + \gamma_1(\alpha_4 e_1 + \alpha_3 e_2 + \gamma_4 e_3 + \gamma_3 e_4) \\ &= (\gamma_1\alpha_4 + \gamma_2\alpha_3 - \gamma_3\alpha_2)e_1 + (\alpha_2 + \gamma_4)\gamma_1 e_3, \end{aligned}$$

which gives

$$\alpha_2 = -\gamma_4, \quad \text{and} \quad \alpha_4 = \frac{1}{\gamma_1^2}\left(\gamma_1 + \gamma_3^2\gamma_2 - 2\gamma_4\gamma_3\gamma_1\right).$$

Then we obtain the matrix in (3.9). Now, note that the following hold:

$$\begin{aligned} Ae_2 &= \alpha_2 e_1 - \gamma_3 e_2 + \gamma_2 e_3 + \gamma_1 e_4, \\ A(\alpha_2 e_1 - \gamma_3 e_2 + \gamma_2 e_3 + \gamma_1 e_4) &= A^2 e_2 = e_1, \\ Ae_1 &= \alpha_1 e_1 + \gamma_1 e_3, \\ A(\alpha_1 e_1 + \gamma_1 e_3) &= A^2 e_1 = 0, \end{aligned}$$

and from $\gamma_1 \neq 0$ it follows that (3.9) has Jordan normal form $J_4(0)$.

If $\gamma_1 = 0$ and $\alpha_3 \neq 0$, then from (3.22) we obtain that $\alpha_1 = \gamma_3 = 0$. Once again we use (3.20) and (3.21) in $A^2 e_2 = e_1$ and then we have $\gamma_2 = \frac{1}{\alpha_3}$. Hence, the square root is

$$\begin{bmatrix} 0 & \alpha_2 & \alpha_3 & \alpha_4 \\ 0 & 0 & 0 & \alpha_3 \\ 0 & \frac{1}{\alpha_3} & 0 & -\alpha_2 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Note that the following hold:

$$\begin{aligned} Ae_4 &= \alpha_4 e_1 + \alpha_3 e_2 + \gamma_4 e_3, \\ A(\alpha_4 e_1 + \alpha_3 e_2 + \gamma_4 e_3) &= A^2 e_4 = e_3, \\ Ae_3 &= \alpha_3 e_1, \\ A(\alpha_3 e_1) &= 0, \end{aligned}$$

and from $\alpha_3 \neq 0$ it follows that (3.10) has Jordan normal form $J_4(0)$.

If $\gamma_1 = \alpha_3 = 0$, then it follows that $Ae_1 = Ae_3 = 0$ which contradicts the equations in (3.21) multiplied by A. $\square$

We remark that the canonical forms found for the square roots in all cases correspond with those given for the H-selfadjoint square roots found in [16, Theorem 3.1].

Agreement. Note that the Jordan normal forms of square roots of all types of pairs in any Segre pairing are uniquely determined, except in the case for $(1,1)$ (the second item of Theorem 3.3.3), where it can be $J_2(0)$ or $J_1(0) \oplus J_1(0)$. But a pair $(1,1)$ in any Segre pairing could just as well be replaced by two pairs $(1,0), (1,0)$, which will also have a square root with Jordan normal form $J_1(0) \oplus J_1(0)$ (the first item of Theorem 3.3.3). Therefore, we agree not to allow $\left[\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right]$ as a square root for a pair $(1,1)$, i.e., we exclude $\alpha = 0$ in (3.7) of Theorem 3.3.3. Thus, under this agreement, we have that the Jordan normal forms corresponding to all pairs in a Segre pairing are uniquely determined.

We say that a square root is *associated with a Segre pairing* if it is a direct sum of square roots associated with each pair of the Segre pairing (see Theorem 3.3.3). All square roots of nilpotent matrices associated with a Segre pairing have the same Jordan normal form.

Then the following result is obtained from Theorem 3.3.3:

Corollary 3.3.4. *Let B_0 be a nilpotent H-nonnegative matrix. Then there is a one-to-one correspondence between the Jordan normal forms of the square roots A_0 of B_0 and the Segre pairings of B_0.*

Thus two different Segre pairings of a matrix B_0 give two different Jordan normal forms of square roots of B_0.

Example 3.3.5. Let $B_0 = J_2(0) \oplus J_2(0) \oplus J_1(0) \oplus J_1(0)$ and $H = Q_2 \oplus Q_2 \oplus \varepsilon_1 Q_1 \oplus \varepsilon_2 Q_1$, where $\varepsilon_1, \varepsilon_2 = \pm 1$. Then B_0 is H-nonnegative, see Theorem 3.2.2. The Segre characteristic of B_0 is $(2, 2, 1, 1)$. There exist three different Segre pairings. Any square root of B_0 which is associated with the Segre pairing $(2, 2), (1, 1)$, will have Jordan normal form $J_4(0) \oplus J_2(0)$. Any square root which is associated with the Segre pairing $(2, 2), (1, 0), (1, 0)$, will have Jordan normal form $J_4(0) \oplus J_1(0) \oplus J_1(0)$, and finally any square root which is associated with the Segre pairing $(2, 1), (2, 1)$, will have Jordan normal form $J_3(0) \oplus J_3(0)$. That is, a Segre pairing identifies the Jordan normal form of a square root, but not the square root itself. There are many square roots related to a Segre pairing, as it is described in Theorem 3.3.3.

Combining the singular and nonsingular cases, we can formulate the following result which presents the Jordan normal form of all square roots. Let $\mathcal{S}$ be any Segre pairing of an H-nonnegative matrix B. Furthermore, let ℓ_1 denote the number of pairs $(1, 0)$ in $\mathcal{S}$, ℓ_2 the number of $(1, 1)$ pairs in $\mathcal{S}$, ℓ_3 the number of $(2, 1)$ pairs in $\mathcal{S}$, and ℓ_4 the number of $(2, 2)$ pairs in $\mathcal{S}$.

Theorem 3.3.6. *Any square root of the H-nonnegative matrix B has the Jordan normal form $A = A_- \oplus A_0 \oplus A_+$ with*

$$A_+ = \bigoplus_{j=1}^{q} J_1(\delta_j \sqrt{\lambda_j}), \quad A_- = \bigoplus_{j=1}^{r-q} J_1(i\delta_{q+j} \sqrt{-\lambda_{q+j}})$$

where $\lambda_1, \ldots, \lambda_q > 0$ and $\lambda_{q+1}, \ldots, \lambda_r < 0$, counting multiplicities, $\delta_j = \pm 1$, and A_0 is given by

$$A_0 = \bigoplus_{i=1}^{\ell_1} J_1(0) \oplus \bigoplus_{i=1}^{\ell_2} J_2(0) \oplus \bigoplus_{i=1}^{\ell_3} J_3(0) \oplus \bigoplus_{i=1}^{\ell_4} J_4(0).$$

The proof is trivial from Theorem 3.3.3 and Corollary 3.3.4.

Note that B_- and B_+ have a lot of square roots as can be seen in the following example.

Example 3.3.7. Let the matrix B be given as

$$B = J_1(-3) \oplus J_1(-3) = \begin{bmatrix} -3 & 0 \\ 0 & -3 \end{bmatrix}.$$

Then the following matrices are some of the square roots of B:

$$\begin{bmatrix} i\sqrt{3} & 0 \\ 0 & i\sqrt{3} \end{bmatrix}, \begin{bmatrix} -i\sqrt{3} & 0 \\ 0 & -i\sqrt{3} \end{bmatrix}, \begin{bmatrix} i\sqrt{3} & 0 \\ 0 & -i\sqrt{3} \end{bmatrix}, \begin{bmatrix} 2i & 1 \\ 1 & -2i \end{bmatrix}, \begin{bmatrix} 2 & -7 \\ 1 & -2 \end{bmatrix}.$$

3.4 H-selfadjoint square roots

Taking Section 3.3 further, we now investigate H-selfadjoint square roots of H-nonnegative matrices B. We assume that the pair (B, H) is in canonical form. Hence by Theorem 3.2.2:

$$B = \bigoplus_{i=1}^{q} J_1(\lambda_i) \oplus \bigoplus_{i=1}^{r-q} J_1(\lambda_{q+i}) \oplus \bigoplus_{i=1}^{s} J_1(0) \oplus \bigoplus_{i=1}^{t} J_2(0),$$

$$H = \bigoplus_{i=1}^{q} Q_1 \oplus \bigoplus_{i=1}^{r-q} (-Q_1) \oplus \bigoplus_{i=1}^{s} \varepsilon_i Q_1 \oplus \bigoplus_{i=1}^{t} Q_2,$$

where $\lambda_1, \ldots, \lambda_q > 0$, $\lambda_{q+1}, \ldots, \lambda_r < 0$, and $\varepsilon_i = \pm 1$. For the following we denote by s_+ (respectively, s_-) the number of positive (respectively, negative) entries in the vector $(\varepsilon_1, \ldots, \varepsilon_s)$, hence we have

$$s = s_- + s_+.$$

Theorem 3.4.1. *Let B be an H-nonnegative matrix in $\mathbb{C}^{n\times n}$. Then B has an H-selfadjoint square root if and only if B satisfies the following:*

(i) *B has no negative eigenvalues, that is, $\sigma(B) \subset [0, \infty)$;*

(ii) *At the eigenvalue zero of B, the number of Jordan blocks of size one with positive sign characteristic is not less than the number of Jordan blocks of size two, i.e.,*

$$s_+ \geq t.$$

Proof. Let B be an H-nonnegative matrix. Note that B is also H-selfadjoint by Theorem 3.2.2. If conditions (i) and (ii) hold, then it follows from Theorem 3.2.3 that B has an H-selfadjoint square root.

Conversely, assume that the H-nonnegative matrix B has an H-selfadjoint square root A. Because of the structure of B as given in Theorem 3.2.2, it follows directly from Theorem 3.2.3 that B cannot have negative eigenvalues. Regarding the second assertion, Theorem 3.2.3 also implies that the blocks corresponding to the pairs $(2, 1)$ in the Segre pairing have the same sign characteristic. In fact, from Theorem 3.2.2, they all have positive sign characteristic. Consider a pair $(2, 2)$ in a Segre pairing of B which comes from $J_2(0) \oplus J_2(0)$. By Theorem 3.2.2 each block has positive sign characteristic, but Theorem 3.2.3 states that for $J_2(0) \oplus J_2(0)$ to have an H-selfadjoint square root, the two blocks must have opposite sign characteristic. This means that a pair $(2, 2)$ can never be a member of any Segre pairing for an H-nonnegative matrix. Consequently, all pairs in a Segre pairing containing a 2 are of the form $(2, 1)$, so there must be in B at least as many Jordan blocks of size one with positive sign characteristic as the number of Jordan blocks of size two. □

Remark 3.4.2. We mention that the "only if" part of Theorem 3.4.1 can also be obtained by using known results on H-plus matrices and H-polar decompositions. Let B be an H-nonnegative matrix. Assume that B has an H-selfadjoint square root A. Then we can write $B = A^{[*]}A$. Since $[Bx, x] \geq 0$ for all $x \in \mathbb{C}^n$ we have from [5] that A is an H-plus matrix since $\mu(A) = \inf_{[u,u]=1}[A^{[*]}Au, u] \geq 0$. The matrix A admits a trivial H-polar decomposition: $A = I \cdot A$. Finally, by part (c) of Theorem 3.4 in [5], see errata in [6], it follows that B has no negative eigenvalues and by part (a) in the same theorem, it follows that $s_+ \geq t$.

We now obtain an explicit description of all H-selfadjoint square roots of a nilpotent H-nonnegative matrix B_0.

Theorem 3.4.3. *Let B_0 be a nilpotent H-nonnegative matrix in Jordan normal form satisfying the second condition in Theorem 3.4.1 and having a Segre pairing $\mathcal{S}$. Any pair of $\mathcal{S}$ is of the form*

$$(2,1),\ (1,1)\ \text{or}\ (1,0). \tag{3.23}$$

This corresponds to Jordan blocks of the form $J_2(0) \oplus J_1(0)$, $J_1(0) \oplus J_1(0)$ and $J_1(0)$, respectively, in the matrix B_0. Then the H-selfadjoint square roots associated with each possible pair in $\mathcal{S}$ are as follows:

(i) *The H-selfadjoint square root of $J_1(0) = [0]$, which is associated with the pair $(1,0)$, is equal to $[0]$. Its Jordan normal form is $J_1(0)$ again.*

(ii) *The H-selfadjoint square roots of $J_1(0) \oplus J_1(0)$, which is associated with the pair $(1,1)$, and where the two blocks have opposite sign characteristic, are of the form*

$$\begin{bmatrix} \alpha & -\bar{\beta} \\ \beta & -\alpha \end{bmatrix}, \text{ for any real } \alpha \text{ and complex } \beta,\ |\beta| = |\alpha|.$$

The Jordan normal form of all matrices of this form is $J_2(0)$.

(iii) *The H-selfadjoint square roots of $J_2(0) \oplus J_1(0)$, which is associated with the pair $(2,1)$, and where the two blocks have both positive sign characteristic, are of the form*

$$\begin{bmatrix} 0 & \alpha & \beta \\ 0 & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \end{bmatrix}, \text{ for real } \alpha \text{ and complex } \beta,\ |\beta| = 1.$$

The Jordan normal form of all matrices of this form is $J_3(0)$.

Proof. Relation (3.23) follows from (3.5) and the fact that a pair $(2,2)$ can never be a member of any Segre pairing for an H-nonnegative matrix, with an H-selfadjoint square root, which was shown in the proof of Theorem 3.4.1.

Assertion (i) is trivial. For (ii) we note that equations (3.6) and (3.7) give the possible forms of square roots in this case. Firstly, for the matrix A as in (3.6), since $J_1(0) \oplus J_1(0)$ is H-selfadjoint where $H = \varepsilon_1 Q_1 \oplus \varepsilon_2 Q_1$, for some $\varepsilon_i = \pm 1$, we see that

$$HA = \begin{bmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{bmatrix} \begin{bmatrix} \alpha & \frac{-\alpha^2}{\beta} \\ \beta & -\alpha \end{bmatrix} = \begin{bmatrix} \varepsilon_1 \alpha & \varepsilon_1 \frac{-\alpha^2}{\beta} \\ \varepsilon_2 \beta & -\varepsilon_2 \alpha \end{bmatrix}$$

is equal to $A^* H = (HA)^*$ if and only if $\alpha \in \mathbb{R}$, $\varepsilon_1 \neq \varepsilon_2$ and $|\beta|^2 = \alpha^2$. This gives the H-selfadjoint square root associated with a pair $(1,1)$, as

$$\begin{bmatrix} \alpha & -\bar{\beta} \\ \beta & -\alpha \end{bmatrix}, \quad \text{where } \alpha \in \mathbb{R},\ |\beta| = |\alpha|.$$

As for (3.7), the matrix $\left[\begin{smallmatrix} 0 & \alpha \\ 0 & 0 \end{smallmatrix}\right]$ is H-selfadjoint if and only if $\alpha = 0$, but we agreed to exclude this case for a pair $(1,1)$, since it is covered by two pairs $(1,0),(1,0)$.

For (iii) we note that $J_2(0) \oplus J_1(0)$ is H-selfadjoint where $H = Q_2 \oplus \varepsilon Q_1$, but from the proof of Theorem 3.4.1 we know that $\varepsilon = 1$. Let A be the matrix in (3.8), which is associated with a pair $(2,1)$. Then we have

$$HA = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & \alpha & \beta \\ 0 & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \alpha & \beta \\ 0 & \frac{1}{\beta} & 0 \end{bmatrix}.$$

This matrix is equal to $A^*H = (HA)^*$ if and only if $\alpha \in \mathbb{R}$ and $|\beta|^2 = 1$. Therefore the H-selfadjoint square root associated with a pair $(2,1)$ is

$$\begin{bmatrix} 0 & \alpha & \beta \\ 0 & 0 & 0 \\ 0 & \frac{1}{\beta} & 0 \end{bmatrix}, \quad \alpha \text{ real}, \ |\beta| = 1. \qquad \square$$

The fact in (ii) of Theorem 3.4.3, that the two blocks in $J_1(0) \oplus J_1(0)$ should have opposite sign characteristic for the existence of an H-selfadjoint square root, also follows from Theorem 3.2.3. Of course, when the blocks $J_1(0)$ in B do not have the correct sign characteristic to be paired as $(1,1)$, they can be paired as two pairs $(1,0),(1,0)$.

For the following result where the canonical form of the H-selfadjoint square roots are given, let $\mathcal{S}$ be any Segre pairing of an H-nonnegative matrix B. Also, let ℓ_1 denote the number of pairs $(1,0)$ in $\mathcal{S}$, ℓ_2 the number of $(1,1)$ pairs in $\mathcal{S}$, and ℓ_3 the number of $(2,1)$ pairs in $\mathcal{S}$. Although not necessary, we may (and do) assume here without loss of generality that (B,H) is in canonical form where B is H-nonnegative.

Theorem 3.4.4. *Let B be an H-nonnegative matrix satisfying the conditions in Theorem 3.4.1. Assume that (B,H) is in canonical form. Then the canonical form of the pair (A,H), where A is an H-selfadjoint square root of B, is given by:*

$$S^{-1}AS = \bigoplus_{i=1}^{q_1} J_1(\sqrt{\lambda_i}) \oplus \bigoplus_{i=1}^{q_2} J_1(-\sqrt{\lambda_i}) \oplus \bigoplus_{i=1}^{\ell_1} J_1(0) \oplus \bigoplus_{i=1}^{\ell_2} J_2(0) \oplus \bigoplus_{i=1}^{\ell_3} J_3(0),$$

$$S^*HS = \bigoplus_{i=1}^{q_1} Q_1 \oplus \bigoplus_{i=1}^{q_2} Q_1 \oplus \bigoplus_{i=1}^{\ell_1} \zeta_i Q_1 \oplus \bigoplus_{i=1}^{\ell_2} \eta_i Q_2 \oplus \bigoplus_{i=1}^{\ell_3} Q_3,$$

for some invertible matrix S, where $q_1 + q_2 = q$, $\lambda_1, \dots, \lambda_q > 0$, the number ζ_i is equal to the sign characteristic of the corresponding block $J_1(0)$ in B, and $\eta_i = \pm 1$.

Proof. As $\sigma(B) \subset [0,\infty)$, see Theorem 3.4.1, the spectrum of A is real. This and Theorem 3.4.3 show the form of $S^{-1}AS$. The sign characteristics related to the blocks $J_1(\sqrt{\lambda_i})$ and $J_1(-\sqrt{\lambda_i})$ follow from part (c) in [16, Theorem 3.1]. The sign characteristics related to the blocks $J_1(0)$, $J_2(0)$ and $J_3(0)$ follow from part (d), (f), and (e), respectively, in [16, Theorem 3.1]. $\square$

3.5 H-nonnegative square roots

In this section we study H-nonnegative square roots of H-nonnegative matrices.

Theorem 3.5.1. *Let B be an H-nonnegative matrix in $\mathbb{C}^{n\times n}$. Then B has an H-nonnegative square root if and only if the following properties hold:*

- (i) *B has no negative eigenvalues, that is, $\sigma(B) \subset [0, \infty)$;*
- (ii) *B has no Jordan blocks of size two at the eigenvalue zero, that is, $t = 0$ in the canonical form of (B, H) as given in Theorem 3.2.2.*

Proof. Suppose that (i) and (ii) hold. Then by Theorem 3.4.1 (also, Theorem 3.2.3) B has an H-selfadjoint square root, say A. The canonical form of (A, H) is given in Theorem 3.4.4 and with $q_2 = 0$, $\ell_3 = 0$ and $\eta_i = 1$ for all $i = 1, \dots, \ell_2$, A is an H-nonnegative square root of B.

Conversely, suppose B has an H-nonnegative square root A. By Theorem 3.4.1 $\sigma(B) \subset [0, \infty)$ and $s_+ \geq t$. But by Theorem 3.2.2 the Jordan normal form of A contains no blocks $J_3(0)$ and $J_4(0)$, which by Theorem 3.3.3 would originate from pairs $(2, 1)$ and $(2, 2)$ in a Segre pairing of B. Therefore, B can have no Jordan blocks of size two at the eigenvalue zero. ☐

Remark 3.5.2. The "only if" direction in Theorem 3.5.1 may also be deduced from [3]. Indeed, suppose B is H-nonnegative, and has an H-nonnegative square root A. Then $B = A^2 = A^{[*]}A$. Moreover, A admits a trivial semidefinite H-polar decomposition: $A = I \cdot A$ in terms of Section 5 in [3]. Hence it follows from Theorem 5.3 in [3] that B has all its eigenvalues in $[0, \infty)$ and is diagonalizable, which implies in particular that the Jordan blocks at zero are all of size one. In fact, from Theorem 5.3 in [3] one extra point may be concluded, namely that $\dim \operatorname{Ker} A \geq \max(s_+, s_-)$.

By Theorem 3.5.1 there exists an H-nonnegative square root for an H-nonnegative matrix B if and only if the canonical form of the pair (B, H) is given by

$$S^{-1}BS = \bigoplus_{i=1}^{q} J_1(\lambda_i) \oplus \bigoplus_{i=1}^{s} J_1(0), \tag{3.24}$$

$$S^{*}HS = \bigoplus_{i=1}^{q} Q_1 \oplus \bigoplus_{i=1}^{s} \varepsilon_i Q_1, \tag{3.25}$$

for some invertible matrix S, where $\lambda_i > 0$ for all $i = 1, \dots, q$ and $\varepsilon_i = \pm 1$ for all $i = 1, \dots, s$. Note that the Segre characteristic of B is equal to $(1, \dots, 1)$. This implies the following theorem.

Theorem 3.5.3. *Let B_0 be a nilpotent H-nonnegative matrix in Jordan normal form satisfying the conditions in Theorem 3.5.1 and having a Segre pairing $\mathcal{S}$. Any pair of $\mathcal{S}$ is of the form*

$$(1, 1) \text{ or } (1, 0).$$

This corresponds to Jordan blocks of the form $J_1(0) \oplus J_1(0)$ and $J_1(0)$, respectively, in the matrix B_0. Then the H-nonnegative square roots associated with each possible pair in $\mathcal{S}$ are given by the first two items in Theorem 3.4.3.

We now also give the canonical form of the H-nonnegative square roots. Let $\mathcal{S}$ be any Segre pairing of an H-nonnegative matrix B. Once again, let ℓ_1 denote the number of pairs $(1,0)$ in $\mathcal{S}$ and ℓ_2 the number of pairs $(1,1)$ in $\mathcal{S}$.

Theorem 3.5.4. *Let B be an H-nonnegative matrix satisfying the conditions in Theorem 3.5.1. Assume that (B,H) is in canonical form, i.e. $S=I$ in (3.24) and (3.25). Then the canonical form of the pair (A,H), where A is an H-nonnegative square root of B, is given by:*

$$P^{-1}AP = \bigoplus_{i=1}^{q} J_1(\sqrt{\lambda_i}) \oplus \bigoplus_{i=1}^{\ell_1} J_1(0) \oplus \bigoplus_{i=1}^{\ell_2} J_2(0),$$

$$P^*HP = \bigoplus_{i=1}^{q} Q_1 \oplus \bigoplus_{i=1}^{\ell_1} \zeta_i Q_1 \oplus \bigoplus_{i=1}^{\ell_2} Q_2,$$

for some invertible matrix P, where ζ_i is equal to the sign characteristic of the corresponding block $J_1(0)$ in B.

Proof. As H-nonnegative square roots of B are also H-selfadjoint, the form of $P^{-1}AP$ follows from Theorem 3.4.4 together with Theorem 3.5.1 and the fact that the H-nonnegative matrix A cannot contain Jordan blocks related with negative eigenvalues of positive sign characteristic, see Theorem 3.2.2. Moreover, Theorem 3.4.4 shows also the sign characteristic related to the blocks $J_1(\sqrt{\lambda_i})$ and $J_1(0)$. The sign characteristic related to $J_2(0)$ was shown in the proof of Theorem 3.5.1. □

3.6 Stability of H-nonnegative square roots

We give a definition for unconditional stability. Later, we relax this definition and consider conditional stability.

Definition 3.6.1. An H-nonnegative square root A of an H-nonnegative matrix B is called *unconditionally stable* if for all $\varepsilon > 0$ there exists a $\delta > 0$ such that for all H-nonnegative matrices $\tilde{B}$ satisfying $\|B - \tilde{B}\| < \delta$, $\tilde{B}$ has an H-nonnegative square root $\tilde{A}$ for which $\|A - \tilde{A}\| < \varepsilon$.

Let B be an H-nonnegative matrix which satisfies the conditions in Theorem 3.5.1. Assume that (B,H) is in canonical form. Let $\mathcal{S}$ be a Segre pairing of the matrix B. Let ℓ_1 be the number of $(1,0)$ pairs in $\mathcal{S}$ and ℓ_2 the number of $(1,1)$ pairs. Then we can write:

$$\begin{aligned} B = B_1 \oplus B_2 \oplus B_3 &= \bigoplus_{i=1}^{\ell_1} J_1(0) \oplus \bigoplus_{i=1}^{\ell_2} (J_1(0) \oplus J_1(0)) \oplus \bigoplus_{i=1}^{q} J_1(\lambda_i), \\ H = H_1 \oplus H_2 \oplus H_3 &= \bigoplus_{i=1}^{\ell_1} \delta_i Q_1 \oplus \bigoplus_{i=1}^{\ell_2} (Q_1 \oplus -Q_1) \oplus \bigoplus_{i=1}^{q} Q_1, \end{aligned} \tag{3.26}$$

where $\lambda_i > 0$, $\delta_i = \pm 1$. Note that by Theorem 3.5.3 the sign characteristics of the different blocks in B are as in Theorem 3.4.3, but this can also be seen from [16, Theorem 3.1].

We follow the proof of [16, Theorem 3.3] for H-selfadjoint square roots with a few adjustments to obtain the following result.

Theorem 3.6.2. *Let B be an H-nonnegative matrix. Then there exists an unconditionally stable H-nonnegative square root of B if and only if in* (3.26)*:*

$$\ell_2 = 0 \quad \text{and} \quad \delta_i = 1. \tag{3.27}$$

Proof. The blocks (B_1, H_1), (B_2, H_2) and (B_3, H_3) can be considered separately. Without loss of generality we can also assume that the matrices B_1, H_1, B_2 and H_2 are of the simplest form, that is, only a single block for B_1 and H_1 and only a single pair of blocks for B_2 and H_2. Consider the matrices $B_1 = J_1(0) = [0]$ (associated with the pair $(1,0)$) and $H_1 = -Q_1 = [-1]$. Then B_1 is H_1-nonnegative. Let $B_1(a) = [-a]$ be a continuous family of matrices with $a \in [0,1]$. Then $B_1(a)$ is H_1-nonnegative and $B_1(0) = B_1$. But $B_1(a)$ does not satisfy the conditions in Theorem 3.5.1 and therefore no H_1-nonnegative square root of $B_1(a)$ exists for $a > 0$. This means that no H_1-nonnegative square root of B_1 is unconditionally stable.

Now consider the matrices $B_2 = J_1(0) \oplus J_1(0) = \left[\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right]$ (associated with the pair $(1,1)$) and

$$H_2 = Q_1 \oplus -Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Let

$$B_2(a) = \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix}, \ a \in [0,1],$$

be a continuous family of matrices. Then $B_2(a)$ is H_2-nonnegative and $B_2(0) = B_2$. Once again, though, $B_2(a)$ does not satisfy the conditions in Theorem 3.5.1. Therefore $B_2(a)$ does not have an H_2-nonnegative square root for $a > 0$ and this means that no H_2-nonnegative square root of B_2 is unconditionally stable. This implies (3.27).

Conversely, let B_3 be an H_3-nonnegative matrix with only positive eigenvalues, thus H_3 is the identity and B_3 is positive definite (see (3.26)). Let Γ be a closed contour which encloses all eigenvalues of B_3 and which lies in the open right half plane. Let $\delta > 0$ be a constant such that all of the eigenvalues of any matrix $\tilde{B}_3$ for which $\|B_3 - \tilde{B}_3\| < \delta$ holds, are enclosed by Γ. Let $\tilde{B}_3$ be an H_3-nonnegative matrix which satisfies $\|B_3 - \tilde{B}_3\| < \delta$. Then $\tilde{B}_3$ is also positive definite. Thus, B_3 and $\tilde{B}_3$ each has a unique positive definite square root A_3 and $\tilde{A}_3$, respectively. Let $\sqrt{\cdot}$ have a branch cut along the negative real line. Then

$$A_3 = \frac{1}{2\pi i} \int_\Gamma \sqrt{z}(zI - B_3)^{-1} dz \quad \text{and} \quad \tilde{A}_3 = \frac{1}{2\pi i} \int_\Gamma \sqrt{z}(zI - \tilde{B}_3)^{-1} dz.$$

Consider

$$A_3 - \tilde{A}_3 = \frac{1}{2\pi i} \int_\Gamma \sqrt{z}[(zI - B_3)^{-1} - (zI - \tilde{B}_3)^{-1}] dz,$$

and note that $(zI - B_3)^{-1} - (zI - \tilde{B}_3)^{-1} = (zI - B_3)^{-1}(B_3 - \tilde{B}_3)(zI - \tilde{B}_3)^{-1}$, then

$$\begin{aligned} \|A_3 - \tilde{A}_3\| &\le \frac{1}{2\pi} \int_\Gamma \left\| \sqrt{z}(zI - B_3)^{-1}(B_3 - \tilde{B}_3)(zI - \tilde{B}_3)^{-1} \right\| |dz| \\ &\le \|B_3 - \tilde{B}_3\| \frac{1}{2\pi} \int_\Gamma |\sqrt{z}| \left\| (zI - B_3)^{-1}(zI - \tilde{B}_3)^{-1} \right\| |dz| . \end{aligned}$$

Since Γ is compact and $(zI - B_3)^{-1}$ is continuous in the entries of B_3, there exists a $\delta > 0$ for all $\varepsilon > 0$ such that $\|B_3 - \tilde{B}_3\| < \delta$ implies

$$\Big| \|(zI - B_3)^{-1}\| - \|(zI - \tilde{B}_3)^{-1}\| \Big| < \varepsilon.$$

Then, using the fact that $\sqrt{z}$ is continuous on Γ (thus, bounded),

$$\begin{aligned} \|A_3 - \tilde{A}_3\| &\leq \|B_3 - \tilde{B}_3\| \frac{1}{2\pi} \int_\Gamma |\sqrt{z}| \left\|(zI - B_3)^{-1}\right\|^2 |dz| \\ &= M\|B_3 - \tilde{B}_3\|, \end{aligned}$$

where M is a constant that only depends on B_3. Therefore we have that the H_3-nonnegative square root A_3 is unconditionally stable.

For the case where $H_1 = Q_1 = [1]$, the matrix B_1 is also H_1-nonnegative and the only square root of B_1 is $A_1 = [0]$. Consider a sequence converging to zero entailing only nonnegative numbers. Now form a sequence by taking the positive square root of each number in that sequence. Then this sequence also converges to zero. This is enough to prove that for every B_k converging to B_1 there exists an H_1-nonnegative square root A_k that converges to A_1, i.e. A_1 is unconditionally stable. ☐

We now define conditional stability to ensure that the matrix close to B admits an H-nonnegative square root.

Definition 3.6.3. An H-nonnegative square root A of an H-nonnegative matrix B is called *conditionally stable* if for all $\varepsilon > 0$ there exists a $\delta > 0$ such that for all H-nonnegative matrices $\tilde{B}$ having at least one H-nonnegative square root, and satisfying $\|B - \tilde{B}\| < \delta$, $\tilde{B}$ has an H-nonnegative square root $\tilde{A}$ for which $\|A - \tilde{A}\| < \varepsilon$.

In the following theorem we find conditions for conditional stability of H-nonnegative square roots of H-nonnegative matrices. Again, we closely follow the proof for H-selfadjoint square roots in [16].

Theorem 3.6.4. *Let B be an H-nonnegative matrix. Then there exists a conditionally stable H-nonnegative square root A of B if and only if in* (3.26)*:*

$$\ell_2 = 0.$$

Proof. Let $B_1 = J_1(0) = [0]$ and $H_1 = \delta Q_1 = [\delta]$, with $\delta = \pm 1$. The only square root of B_1 is $A_1 = [0]$. If $\delta = 1$, by Theorem 3.6.2, A_1 is unconditionally stable and, hence also conditionally stable. If $\delta = -1$, the only H_1-nonnegative matrix having an H_1-nonnegative square root, is the zero matrix. Therefore, consider the constant sequence $0, 0, \ldots$. Then it follows that the H_1-nonnegative square root A_1 is conditionally stable.

Next, let $B_2 = J_1(0) \oplus J_1(0)$ and $H_2 = Q_1 \oplus -Q_1$. We know from Theorem 3.5.3 that any H_2-nonnegative square root of B_2 is of the form

$$A_2 = \begin{bmatrix} \alpha & -\bar{\beta} \\ \beta & -\alpha \end{bmatrix} \text{ for any } \alpha \in \mathbb{R},\ \beta \in \mathbb{C} \text{ with } |\beta| = \pm\alpha.$$

Note that, according to the Agreement in Section 3.3, we always consider $\alpha \neq 0$. Consider a continuous family of H_2-nonnegative matrices:

$$B(a) = \begin{bmatrix} a & 0 \\ 0 & 0 \end{bmatrix}, \ a \in [0, 1].$$

The only H_2-nonnegative square root of $B(a)$ is $\left[\begin{smallmatrix} \sqrt{a} & 0 \\ 0 & 0 \end{smallmatrix}\right]$ but this matrix converges to the zero matrix (and not A_2) as a converges to 0. Therefore, no H_2-nonnegative square root of B_2 is conditionally stable.

Lastly, let B_3 be an H_3-nonnegative matrix with only positive eigenvalues. By Theorem 3.6.2 there exists an unconditionally stable H_3-nonnegative square root A_3 which is then also conditionally stable. $\square$

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Chapter 4

Quaternion H-selfadjoint mth roots[1]

Abstract. The complex matrix representation for a quaternion matrix is used in this chapter to find necessary and sufficient conditions for the existence of an H-selfadjoint mth root of a given H-selfadjoint quaternion matrix. In the process, when such an H-selfadjoint mth root exists, its construction is also given.

Keywords. Quaternion matrices, Roots of matrices, Indefinite inner product, H-selfadjoint matrices, Canonical forms.
AMS subject classifications. 15B33, 15A16, 47B50.

4.1 Introduction

Denote the skew field of real quaternions by $\mathbb{H}$. The basic theory of quaternion linear algebra can be found in various books and papers, see for example the book by Leiba Rodman [10], and [13, 14]. Let m be any positive integer and let H be a square quaternion matrix which is invertible and Hermitian. We focus on the class of selfadjoint matrices relative to the indefinite inner product generated by H. In the general sense of the definition, a square quaternion matrix A is said to be H-selfadjoint if $HA = A^*H$.

If B is a square H-selfadjoint matrix with quaternion entries, we seek to find necessary and sufficient conditions for the existence of an H-selfadjoint matrix A such that $A^m = B$. This matrix A is referred to as an H-selfadjoint mth root of the matrix B.

It is well known that there exists a complex matrix representation for a matrix with quaternion entries, that is, there exists an isomorphism ω_n between the real algebra of all $n \times n$ quaternion matrices and a subalgebra Ω_{2n} of the algebra of all $2n \times 2n$ complex matrices. The isomorphism ω_n maps an $n \times n$ quaternion matrix $A = A_1 + \mathrm{j}A_2$, where $A_1, A_2 \in \mathbb{C}^{n\times n}$, to a $2n \times 2n$ matrix:

$$\begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix}.$$

This fact simplifies our problem. Therefore, we find necessary and sufficient conditions for the existence of an $\tilde{H}$-selfadjoint mth root in Ω_{2n} of an $\tilde{H}$-selfadjoint matrix in Ω_{2n}.

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Quaternion matrices in indefinite inner product spaces, and specifically different canonical forms, were studied in [1, 4, 9, 11]. Not much research has been done on roots of quaternion matrices, although [7] does give a formula for obtaining mth roots of quaternion matrices of a particular form. On the other hand, in the complex case, H-selfadjoint mth roots of H-selfadjoint matrices have been studied extensively. Necessary and sufficient conditions for the existence of such roots can be found in [5][2]. For the case of H-selfadjoint square roots and applications to polar decompositions of H-selfadjoint matrices, see [2], and for the case of square roots of H-nonnegative matrices, see [8][3]. We refer to the introduction of a previous paper [5][2], for an overview of mth roots of matrices in general.

Note that in the process of finding an H-selfadjoint mth root $A \in \Omega_{2n}$ of $B \in \Omega_{2n}$, the functional analytic approach via the Cauchy integral:

$$A := \frac{1}{2\pi \mathsf{i}} \int_{\Gamma} \sqrt[m]{\lambda} (\lambda I - B)^{-1} \, d\lambda,$$

which can be found for example in [6], would be sufficient in the case where there are no eigenvalues of B in $(-\infty, 0]$. However, in this chapter, we prefer to take a more direct approach also in the case where the eigenvalues do not lie on the negative real line.

4.2 Preliminaries

We recap the basic theory for quaternions and matrices with quaternion entries as found in the book by Leiba Rodman [10]. Every element in $\mathbb{H}$ is of the form:

$$x = x_0 + x_1\mathsf{i} + x_2\mathsf{j} + x_3\mathsf{k},$$

where $x_0, x_1, x_2, x_3 \in \mathbb{R}$ and the elements $\mathsf{i}, \mathsf{j}, \mathsf{k}$ satisfy the following formulas:

$$\mathsf{i}^2 = \mathsf{j}^2 = \mathsf{k}^2 = -1, \quad \mathsf{ij} = -\mathsf{ji} = \mathsf{k}, \quad \mathsf{jk} = -\mathsf{kj} = \mathsf{i}, \quad \mathsf{ki} = -\mathsf{ik} = \mathsf{j}.$$

It is important to keep in mind the fact that multiplication in $\mathbb{H}$ is not commutative, that is, in general $xy \neq yx$ for $x, y \in \mathbb{H}$. Let $\bar{x} = x_0 - x_1\mathsf{i} - x_2\mathsf{j} - x_3\mathsf{k}$ denote the conjugate quaternion of x. For a quaternion matrix A, let $\bar{A}$ denote the matrix in which each entry is the conjugate of the corresponding entry in A.

Let A be an $n \times n$ quaternion matrix, that is, $A \in \mathbb{H}^{n\times n}$, and write A as $A = A_1 + \mathsf{j}A_2$ where $A_1, A_2 \in \mathbb{C}^{n\times n}$. The map $\omega_n : \mathbb{H}^{n\times n} \to \mathbb{C}^{2n\times 2n}$ is defined by:

$$\omega_n(A) = \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix}.$$

Then ω_n is an isomorphism of the real algebra $\mathbb{H}^{n\times n}$ onto the real unital subalgebra

$$\Omega_{2n} := \left\{ \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix} \mid A_1, A_2 \in \mathbb{C}^{n\times n} \right\}$$

of $\mathbb{C}^{2n\times 2n}$. The following properties can be found in [10, Section 3.4] and [13]. Let $X, Y \in \mathbb{H}^{n\times n}$ and $s, t \in \mathbb{R}$ be arbitrary, then

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[2] Included in this thesis as Chapter 2.

[3] Included in this thesis as Chapter 3.

(i) $\omega_n(I_n) = I_{2n}$;

(ii) $\omega_n(XY) = \omega_n(X)\omega_n(Y)$;

(iii) $\omega_n(sX + tY) = s\omega_n(X) + t\omega_n(Y)$;

(iv) $\omega_n(X^*) = (\omega_n(X))^*$;

(v) X is invertible if and only if $\omega_n(X)$ is invertible; if so, then $\omega_n(X^{-1}) = (\omega_n(X))^{-1}$.

Note that the matrix $X^* \in \mathbb{H}^{n\times m}$ is obtained from $X \in \mathbb{H}^{m\times n}$ by replacing each entry with its conjugate quaternion and then taking the transpose. This isomorphism between $\mathbb{H}^{n\times n}$ and Ω_{2n} ensures that results for matrices in $\mathbb{H}^{n\times n}$ that are purely algebraic are also true for matrices in the subalgebra Ω_{2n} since we can apply ω_n, and vice versa as long as we stay within the subalgebra Ω_{2n}. All definitions that follow could also be made with respect to matrices in Ω_{2n}.

An $n \times n$ quaternion matrix A has left eigenvalues and right eigenvalues but since we only work with right eigenvalues and right eigenvectors, we will refer to them as *eigenvalues* and *eigenvectors*.

Definition 4.2.1. A nonzero vector $v \in \mathbb{H}^n$ is called an *eigenvector* of a matrix $A \in \mathbb{H}^{n\times n}$ corresponding to the *eigenvalue* $\lambda \in \mathbb{H}$ if the equality $Av = v\lambda$ holds.

The *spectrum* of A, denoted by $\sigma(A)$, is the set of all eigenvalues of A. Note that $\sigma(A)$ is closed under similarity of quaternions, that is, if v is an eigenvector of A corresponding to the eigenvalue λ, then $v\alpha$ is an eigenvector of A corresponding to the eigenvalue $\alpha^{-1}\lambda\alpha$, for all nonzero $\alpha \in \mathbb{H}$. From [13] we see that A has exactly n eigenvalues which are complex numbers with nonnegative imaginary parts, multiplicity taken into account. All eigenvalues of A are obtained from these n complex eigenvalues with nonnegative imaginary parts by quaternion conjugation, and the Jordan normal form of A has exactly these numbers on the diagonal. Let $\mathbb{C}_+ = \{a + \mathrm{i}b \mid a \in \mathbb{R},\, b > 0\}$.

Let a single Jordan block of size $n \times n$ at the eigenvalue λ be denoted by $J_n(\lambda)$. The $n \times n$ matrix with ones on the main anti-diagonal and zeros elsewhere, called a standard involutory permutation (sip) matrix, is denoted by Q_n.

Recall the following definition from [12].

Definition 4.2.2. Let A be a square quaternion matrix with Jordan blocks $\bigoplus_{i=1}^{r} J_{n_i}(\lambda)$ at the eigenvalue λ in its Jordan normal form and assume that $n_1 \geq n_2 \geq n_3 \geq \ldots \geq n_r > 0$. The *Segre characteristic* of A corresponding to the eigenvalue λ is defined as the sequence:

$$n_1, n_2, n_3, \ldots, n_r, 0, 0, \ldots .$$

We will use this definition mostly in the case where λ is equal to zero unless indicated otherwise and therefore sometimes will simply use *Segre characteristic* to refer to the Segre characteristic of A corresponding to the eigenvalue 0. Note that the Jordan normal form of matrices in the subalgebra Ω_{2n} can be found from the Jordan normal form of matrices in $\mathbb{H}^{n\times n}$ since $\omega_n(J_n(\lambda)) = J_n(\lambda) \oplus J_n(\bar{\lambda})$, for $\lambda \in \mathbb{C}$. Then it is easy to see the following result.

Corollary 4.2.3. *If a nilpotent matrix A is in Ω_{2n}, then each number in the Segre characteristic of A occurs twice.*

This actually holds for the Segre characteristic corresponding to any real eigenvalue in the case where $A \in \Omega_{2n}$ has real numbers in its spectrum. However, only the nilpotent case will be used later.

A matrix $X \in \mathbb{H}^{n\times n}$ is said to be *Hermitian* if $X^* = X$. Let $H \in \mathbb{H}^{n\times n}$ be an invertible Hermitian matrix. We consider the indefinite inner product $[\,\cdot\,,\cdot\,]$ generated by H:

$$[x, y] = \langle Hx, y\rangle = y^* Hx, \quad x, y \in \mathbb{H}^n,$$

where $\langle\cdot\,,\cdot\rangle$ denotes the standard inner product. A matrix $A \in \mathbb{H}^{n\times n}$ is called *H-selfadjoint* if $HA = A^*H$. Two pairs of matrices (A_1, H_1) and (A_2, H_2) are said to be *unitarily similar* if there exists an invertible quaternion matrix S such that $S^{-1}A_1S = A_2$ and $S^*H_1S = H_2$ hold.

As in the complex case, there exists a canonical form for the pair (A, H) where $A \in \mathbb{H}^{n\times n}$ is an H-selfadjoint matrix. This is given in, for example [1, Theorem 4.1], [9] and [10, Theorem 10.1.1].

Theorem 4.2.4. *Let $H \in \mathbb{H}^{n\times n}$ be an invertible Hermitian matrix and $A \in \mathbb{H}^{n\times n}$ an H-selfadjoint matrix. Then there exists an invertible matrix $S \in \mathbb{H}^{n\times n}$ such that*

$$\begin{aligned} S^{-1}AS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus \begin{bmatrix} J_{k_{\alpha+1}}(\lambda_{\alpha+1}) & 0 \\ 0 & J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\lambda_\beta) & 0 \\ 0 & J_{k_\beta}(\overline{\lambda}_\beta) \end{bmatrix}, \end{aligned} \tag{4.1}$$

where $\lambda_i \in \sigma(A) \cap \mathbb{R}$ for all $i = 1, \dots, \alpha$, $\lambda_i \in \sigma(A) \cap \mathbb{C}_+$ for all $i = \alpha + 1, \dots, \beta$, and

$$S^*HS = \eta_1 Q_{k_1} \oplus \cdots \oplus \eta_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \tag{4.2}$$

where $\eta_i = \pm 1$. The form $(S^{-1}AS,\ S^*HS)$ in (4.1) and (4.2) is uniquely determined by the pair (A, H), up to a permutation of diagonal blocks.

We refer to the pair $(S^{-1}AS, S^*HS)$ in (4.1) and (4.2) as the *canonical form* of the pair (A, H) of quaternion matrices.

The following result from [5][4] holds for quaternion matrices as well, but by applying ω_n it also holds for matrices in the subalgebra Ω_{2n}. We use it in the proofs throughout this chapter.

Lemma 4.2.5. *Let X and Y be $n \times n$ quaternion matrices such that the pair (X, H_X) is unitarily similar to the pair (Y, H_Y) where $H_X \in \mathbb{H}^{n\times n}$ and $H_Y \in \mathbb{H}^{n\times n}$ are invertible Hermitian matrices, that is, there exists an invertible matrix $P \in \mathbb{H}^{n\times n}$ such that*

$$P^{-1}XP = Y \quad \text{and} \quad P^*H_XP = H_Y.$$

Let the matrix $J \in \mathbb{H}^{n\times n}$ be an H_X-selfadjoint mth root of X, that is, $J^m = X$. Then the matrix $A := P^{-1}JP$ is an H_Y-selfadjoint mth root of Y.

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[4] Included in this thesis as Chapter 2. The specific reference is to Lemma 2.2.1.

From the properties of the map ω_n, we see that a matrix A is invertible if and only if $\omega_n(A)$ is invertible. Also, from Proposition 3.4.1 in [10], A is Hermitian if only if $\omega_n(A)$ is Hermitian.

To find a canonical form for a pair $(\tilde{A}, \tilde{H})$ where $\tilde{A} \in \Omega_{2n}$ is $\tilde{H}$-selfadjoint, and $\tilde{H} \in \Omega_{2n}$ is invertible and Hermitian, we apply ω_n to the equations (4.1) and (4.2). Denote the right-hand side of (4.1) by J and the right-hand side of (4.2) by Q and then we have

$$(\omega_n(S))^{-1}\omega_n(A)\omega_n(S) = \omega_n(J), \quad \omega_n(S)^*\omega_n(H)\omega_n(S) = \omega_n(Q).$$

The uniqueness follows from the fact that the canonical form of (A, H) is unique (Theorem 4.2.4) and that ω_n is an isomorphism. Therefore, the canonical form of a pair of matrices in Ω_{2n} is as follows.

Theorem 4.2.6. *Let $\tilde{H} \in \Omega_{2n}$ be an invertible Hermitian matrix and $\tilde{A} \in \Omega_{2n}$ an $\tilde{H}$-selfadjoint matrix. Then there exists an invertible matrix $S \in \Omega_{2n}$ such that $S^{-1}\tilde{A}S$ is equal to*

$$\begin{aligned} &J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \oplus \begin{bmatrix} J_{k_{\alpha+i}}(\lambda_{\alpha+i}) & 0 \\ 0 & J_{k_{\alpha+i}}(\overline{\lambda}_{\alpha+i}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\lambda_\beta) & 0 \\ 0 & J_{k_\beta}(\overline{\lambda}_\beta) \end{bmatrix} \oplus \\ &J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \oplus \begin{bmatrix} J_{k_{\alpha+i}}(\overline{\lambda}_{\alpha+i}) & 0 \\ 0 & J_{k_{\alpha+i}}(\lambda_{\alpha+i}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\overline{\lambda}_\beta) & 0 \\ 0 & J_{k_\beta}(\lambda_\beta) \end{bmatrix}, \end{aligned} \tag{4.3}$$

where $\lambda_i \in \sigma(\tilde{A}) \cap \mathbb{R}$ for all $i = 1, \ldots, \alpha$, $\lambda_i \in \sigma(\tilde{A}) \cap \mathbb{C}_+$ for all $i = \alpha + 1, \ldots, \beta$; and

$$\begin{aligned} S^*\tilde{H}S = {} & \eta_1 Q_{k_1} \oplus \cdots \oplus \eta_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta} \\ & \oplus \eta_1 Q_{k_1} \oplus \cdots \oplus \eta_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \end{aligned} \tag{4.4}$$

where $\eta_i = \pm 1$. The form $(S^{-1}\tilde{A}S, S^*\tilde{H}S)$ in (4.3) and (4.4) is uniquely determined by the pair $(\tilde{A}, \tilde{H})$ up to a permutation of diagonal blocks.

We note at this stage that the canonical form of the nonreal part of an H-selfadjoint matrix A must be of dimension a multiple of 4 due to the direct sums of $J_{k_i}(\lambda_i)$ and $J_{k_i}(\overline{\lambda}_i)$ occurring twice. It is crucial to ensure that all matrices throughout the proofs are in Ω_{2n} and for this reason we give the following result to explain why we can study different Jordan blocks separately.

Lemma 4.2.7. *Let $H_1 = R_1 \oplus \bar{R}_1, B_1 = J_1 \oplus \bar{J}_1 \in \Omega_{2n}$ and $H_2 = R_2 \oplus \bar{R}_2, B_2 = J_2 \oplus \bar{J}_2 \in \Omega_{2p}$ where B_1 is H_1-selfadjoint and B_2 is H_2-selfadjoint. Let $A_1 \in \Omega_{2n}$ be an H_1-selfadjoint mth root of B_1 and $A_2 \in \Omega_{2p}$ an H_2-selfadjoint mth root of B_2, and let their entries be as follows:*

$$A_1 = \begin{bmatrix} A_{11}^{(1)} & \bar{A}_{12}^{(1)} \\ -A_{12}^{(1)} & \bar{A}_{11}^{(1)} \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} A_{11}^{(2)} & \bar{A}_{12}^{(2)} \\ -A_{12}^{(2)} & \bar{A}_{11}^{(2)} \end{bmatrix}.$$

Let $\hat{B} = J_1 \oplus J_2 \oplus \bar{J}_1 \oplus \bar{J}_2 \in \Omega_{2(n+p)}$ and $\hat{H} = R_1 \oplus R_2 \oplus \bar{R}_1 \oplus \bar{R}_2 \in \Omega_{2(n+p)}$. Then $\hat{B}$ is $\hat{H}$-selfadjoint and the following matrix $\hat{A}$ is an $\hat{H}$-selfadjoint mth root of the matrix $\hat{B}$:

$$\hat{A} = \begin{bmatrix} A_{11}^{(1)} & 0 & \bar{A}_{12}^{(1)} & 0 \\ 0 & A_{11}^{(2)} & 0 & \bar{A}_{12}^{(2)} \\ -A_{12}^{(1)} & 0 & \bar{A}_{11}^{(1)} & 0 \\ 0 & -A_{12}^{(2)} & 0 & \bar{A}_{11}^{(2)} \end{bmatrix} \in \Omega_{2(n+p)}.$$

Proof. Let P be the following permutation matrix:

$$P = \begin{bmatrix} I_n & 0 & 0 & 0 \\ 0 & 0 & I_p & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_p \end{bmatrix}.$$

This P produces a map from $\Omega_{2n} \oplus \Omega_{2p}$ to $\Omega_{2(n+p)}$ which satisfies $P(A_1 \oplus A_2)P^{-1} = \hat{A}$. We also then have $P(B_1 \oplus B_2)P^{-1} = \hat{B}$ and $P(H_1 \oplus H_2)P^{-1} = \hat{H}$. Therefore,

$$\hat{A}^m = \left(P(A_1 \oplus A_2)P^{-1}\right)^m = P(A_1 \oplus A_2)^m P^{-1} = P(B_1 \oplus B_2)P^{-1} = \hat{B}.$$

Now, by noting that $P^* = P^{-1}$ and using the facts that B_1 and A_1 are H_1-selfadjoint and B_2 and A_2 are H_2-selfadjoint, it follows that $\hat{H}\hat{B} = \hat{B}^*\hat{H}$ and $\hat{H}\hat{A} = \hat{A}^*\hat{H}$. Therefore, $\hat{A}$ is an $\hat{H}$-selfadjoint mth root of the $\hat{H}$-selfadjoint matrix $\hat{B}$. □

The matrix J_i in Lemma 4.2.7 can be the Jordan normal form $J_k(\lambda)$ in the case where λ is real or the Jordan normal form $J_k(\lambda) \oplus J_k(\bar{\lambda})$ in the case where λ is nonreal.

In general, let the permutation matrix P be a $2t \times 2t$ block matrix where the block in the ith row and jth column is defined by:

$$P_{ij} = \begin{cases} I_{2k_i} & \text{if } j = 2i-1,\ i \leq t; \\ I_{2k_{i-t}} & \text{if } j = 2(i-t),\ i > t; \\ 0 & \text{otherwise.} \end{cases} \tag{4.5}$$

Then we have, for example, that

$$P \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j} \oplus Q_{k_j} \oplus -Q_{k_j}\right) P^{-1} = \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j}\right) \oplus \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j}\right).$$

4.3 Existence of mth roots

We first present a very handy tool for working with quaternion matrices.

Lemma 4.3.1. *Let H be an $n \times n$ quaternion matrix which is invertible and Hermitian, and let B be an $n \times n$ H-selfadjoint quaternion matrix. There exists an H-selfadjoint quaternion matrix A such that $A^m = B$ if and only if there exists an $\tilde{H} = \omega_n(H)$-selfadjoint matrix $\tilde{A} = \omega_n(A)$ such that $\tilde{A}^m = \tilde{B}$, where $\tilde{B} = \omega_n(B)$ is an $\tilde{H}$-selfadjoint matrix in the subalgebra Ω_{2n}.*

Proof. From the properties of the map ω_n and the fact that it is an isomorphism from $\mathbb{H}^{n\times n}$ to Ω_{2n}, we see that $A^m = B$ if and only if $(\omega_n(A))^m = \omega_n(B)$, and A is H-selfadjoint if and only if $\omega_n(A)$ is $\omega_n(H)$-selfadjoint. □

Because of this lemma, necessary and sufficient conditions for the existence of an H-selfadjoint mth root of an H-selfadjoint matrix B are the same as the necessary and sufficient conditions for the existence of an $\tilde{H}$-selfadjoint mth root of an $\tilde{H}$-selfadjoint matrix $\tilde{B}$ where $\tilde{B}, \tilde{H} \in \Omega_{2n}$. If we could work in $\mathbb{C}^{2n\times 2n}$, we would now be done by simply referring to [5][5]. However, since ω_n is an isomorphism between $\mathbb{H}^{n\times n}$ and the subalgebra Ω_{2n} of $\mathbb{C}^{2n\times 2n}$, we have to be more careful.

We now first present in Theorem 4.3.2 our main theorem for the existence of H-selfadjoint mth roots of H-selfadjoint matrices in Ω_{2n}. The proof of this theorem may be split into the following separate parts due to Lemma 4.2.7, viz. the case where $\tilde{B}$ has only positive eigenvalues, the case where $\tilde{B}$ has only nonreal eigenvalues, the case where $\tilde{B}$ has only negative eigenvalues (separated into two cases for m even and for m odd), and lastly, the case where $\tilde{B}$ has only zero as an eigenvalue. These we state and prove in Theorems 4.3.3, 4.3.4, 4.3.6, 4.3.7 and 4.3.9.

Theorem 4.3.2. *Let $\tilde{B}$ and $\tilde{H}$ be matrices in the subalgebra Ω_{2n} such that $\tilde{H}$ is invertible and Hermitian, and $\tilde{B}$ is $\tilde{H}$-selfadjoint. Then there exists an $\tilde{H}$-selfadjoint matrix in Ω_{2n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$ if and only if the canonical form of $(\tilde{B}, \tilde{H})$ has the following properties:*

1. *When m is even, the part of the canonical form corresponding to the negative eigenvalues, say $(\tilde{B}_-, \tilde{H}_-)$, is given by*

$$\tilde{B}_- = \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j)\right) \oplus \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j)\right),$$

$$\tilde{H}_- = \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j}\right) \oplus \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j}\right),$$

   where $\lambda_j < 0$.

2. *The part of the canonical form corresponding to the zero eigenvalue, say $(\tilde{B}_0, \tilde{H}_0)$, is given by*

$$\tilde{B}_0 = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=r_j+1}^{m} J_{a_j}(0) \right) \oplus \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=r_j+1}^{m} J_{a_j}(0) \right)$$

   and

$$\tilde{H}_0 = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right) \oplus \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right),$$

   for some $a_j, r_j \in \mathbb{Z}$ with $0 < r_j \leq m$. The signs are as follows, given in terms of η_j, where η_j could be either 1 or -1: If r_j (respectively $m - r_j$) is even, half of $\varepsilon_i^{(j)}$ for $i = 1, \ldots, r_j$ (respectively for $i = r_j + 1, \ldots, m$) are equal to η_j and the other half are equal to $-\eta_j$. If r_j (respectively $m - r_j$) is odd, there is one more of the $\varepsilon_i^{(j)}$ for $i = 1, \ldots, r_j$ (respectively for $i = r_j + 1, \ldots, m$) equal to η_j than to $-\eta_j$.

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[5] Included in this thesis as Chapter 2.

Note that it follows from Lemma 4.2.5 (which also holds for matrices in Ω_{2n}) that it is sufficient to assume that the pair $(\tilde{B}, \tilde{H})$ is in canonical form.

For the positive eigenvalue case, we now prove the following:

Theorem 4.3.3. *Let $\tilde{B}, \tilde{H} \in \Omega_{2n}$, where $\tilde{H}$ is invertible and Hermitian, and $\tilde{B}$ is $\tilde{H}$-selfadjoint with a spectrum consisting of only positive real numbers. Then there exists an $\tilde{H}$-selfadjoint matrix in Ω_{2n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$.*

Proof. Let $\tilde{B} \in \Omega_{2n}$ be $\tilde{H}$-selfadjoint with only positive real eigenvalues, where $\tilde{H} \in \Omega_{2n}$ is invertible and Hermitian. We can assume that $\tilde{B} = J_n(\lambda) \oplus J_n(\lambda)$, where λ is a positive real number, and that $\tilde{H} = \varepsilon Q_n \oplus \varepsilon Q_n$, $\varepsilon = \pm 1$. To construct an mth root of $\tilde{B}$ which is $\tilde{H}$-selfadjoint and also in Ω_{2n}, we let $J = J_n(\mu) \oplus J_n(\mu)$ where μ is the positive real mth root of λ. Then both J and $J^m = (J_n(\mu))^m \oplus (J_n(\mu))^m$ are $\tilde{H}$-selfadjoint, and the Jordan normal form of J^m is equal to $\tilde{B}$. We now wish to find an invertible matrix $P \in \Omega_{2n}$ such that equations

$$P^{-1} J^m P = \tilde{B} \quad \text{and} \quad P^* \tilde{H} P = \tilde{H} \tag{4.6}$$

hold. To ensure that the first equation holds, let $P = P_1 \oplus P_2$ with

$$\begin{aligned} P_1 &= \left[((J_n(\mu))^m - \lambda I)^{n-1} y \quad \cdots \quad ((J_n(\mu))^m - \lambda I) y \quad y \right], \\ P_2 &= \left[((J_n(\mu))^m - \lambda I)^{n-1} z \quad \cdots \quad ((J_n(\mu))^m - \lambda I) z \quad z \right], \end{aligned}$$

where $y, z \in \operatorname{Ker} ((J_n(\mu))^m - \lambda I)^n = \mathbb{C}^n$ but $y, z \notin \operatorname{Ker} ((J_n(\mu))^m - \lambda I)^{n-1}$. From the choices of y and z, it is clear that P_1 and P_2 are invertible $n \times n$ matrices and hence the $2n \times 2n$ matrix P is invertible. Let $z = \bar{y}$, so that $P_2 = \bar{P}_1$; then P is in Ω_{2n}. Note that $P^* \tilde{H} P = \tilde{H}$ if and only if $P_1^* Q_n P_1 = Q_n$ and since $P_1^* Q_n P_1$ is a lower anti-triangular Hankel matrix, $P^* \tilde{H} P = \tilde{H}$ holds if and only if

$$\phi_{n,j}(y) = [p_j, p_n] = y^* Q_n ((J_n(\mu))^m - \lambda I)^{n-j} y = \begin{cases} 1 & \text{if } j = 1, \\ 0 & \text{if } j = 2, \ldots, n, \end{cases}$$

where $\phi_{i,j}(y)$ denotes the entries in the matrix $P_1^* Q_n P_1$ and p_i denotes the columns in the matrix P_1. As illustrated in [5][6], one can easily find one solution to these equations by assuming that y is real. Therefore, there exists a matrix $P \in \Omega_{2n}$ satisfying the equations (4.6). Then by using Lemma 4.2.5, the matrix $\tilde{A} := P^{-1} J P$ is an $\tilde{H}$-selfadjoint mth root of $\tilde{B}$, and $\tilde{A}$ is also in Ω_{2n} since P is. □

Now, for the nonreal eigenvalue case.

Theorem 4.3.4. *Let $\tilde{B}, \tilde{H} \in \Omega_{4n}$, where $\tilde{H}$ is invertible and Hermitian, and $\tilde{B}$ is $\tilde{H}$-selfadjoint with a spectrum consisting of only nonreal numbers. Then there exists an $\tilde{H}$-selfadjoint matrix in Ω_{4n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$.*

Proof. Let $\tilde{B} \in \Omega_{4n}$ be $\tilde{H}$-selfadjoint with only nonreal eigenvalues, where $\tilde{H} \in \Omega_{4n}$ is invertible and Hermitian. We can assume that $\tilde{B} = J_n(\lambda) \oplus J_n(\bar{\lambda}) \oplus J_n(\bar{\lambda}) \oplus J_n(\lambda)$, where λ is a nonreal number, and that $\tilde{H} = Q_{2n} \oplus Q_{2n}$. To construct an mth root of

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[6] Included in this thesis as Chapter 2.

$\tilde{B}$, let $J = J_n(\mu) \oplus J_n(\bar{\mu}) \oplus J_n(\bar{\mu}) \oplus J_n(\mu)$ where μ is any mth root of λ. Then the Jordan normal form of J^m is equal to $\tilde{B}$, and both J and J^m are $\tilde{H}$-selfadjoint. Let $P = P_1 \oplus \bar{P}_1 \oplus \bar{P}_1 \oplus P_1 \in \Omega_{4n}$ where

$$P_1 = \left[((J_n(\mu))^m - \lambda I)^{n-1} y \quad \cdots \quad ((J_n(\mu)^m - \lambda I) y \quad y \right],$$

with $y \in \operatorname{Ker}((J_n(\mu))^m - \lambda I)^n = \mathbb{C}^n$ but $y \notin \operatorname{Ker}((J_n(\mu))^m - \lambda I)^{n-1}$. Then $P^* \tilde{H} P = \tilde{H}$ if and only if $P_1^T Q_n P_1 = Q_n$, and according to the proof of Theorem 2.4 in [5][7], there exists a solution to the latter equation. Hence, there exists an invertible matrix $P \in \Omega_{4n}$ such that the equations

$$P^{-1} J^m P = \tilde{B} \quad \text{and} \quad P^* \tilde{H} P = \tilde{H}$$

hold. Once again, by Lemma 4.2.5, the matrix $\tilde{A} := P^{-1} J P$ is an $\tilde{H}$-selfadjoint mth root of $\tilde{B}$ and is in Ω_{4n}. □

Before stating the results for the negative case, we give the following result which was obtained by applying ω_n to all matrices in Lemma 2.12 of [5][8].

Lemma 4.3.5. *Let $T \in \Omega_{2n}$ be a diagonal block matrix consisting of an upper triangular Toeplitz matrix with diagonal entries $t_1, \ldots, t_n$, and its complex conjugate. Let the diagonal entries $\lambda = t_1$ be real, t_2 nonzero and $B = T \oplus \bar{T}$. Then B is $(Q_{2n} \oplus Q_{2n})$-selfadjoint, and the pair $(B,\, Q_{2n} \oplus Q_{2n})$ is unitarily similar to*

$$(J_n(\lambda) \oplus J_n(\lambda) \oplus J_n(\lambda) \oplus J_n(\lambda),\; Q_n \oplus -Q_n \oplus Q_n \oplus -Q_n).$$

Turning to the case of the negative eigenvalue for a matrix $\tilde{B}$, we first point out that if m is even, any mth root $\tilde{A}$ will necessarily have only nonreal eigenvalues, so in order for $\tilde{A}$ to be $\tilde{H}$-selfadjoint, by Theorem 4.2.6, it (and so also $\tilde{B}$) would have to be in Ω_{4n}. We first prove a result for m even.

Theorem 4.3.6. *Let $\tilde{H} \in \Omega_{4n}$ be an invertible Hermitian matrix and let $\tilde{B} \in \Omega_{4n}$ be an $\tilde{H}$-selfadjoint matrix with a spectrum consisting of only negative real numbers. Then, for an even positive integer m, there exists an $\tilde{H}$-selfadjoint matrix in Ω_{4n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$ if and only if the canonical form of $(\tilde{B}, \tilde{H})$ is given by*

$$S^{-1} \tilde{B} S = \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \right) \oplus \bigoplus_{j=1}^{t} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \right), \tag{4.7}$$

and

$$S^* \tilde{H} S = \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j} \right) \oplus \bigoplus_{j=1}^{t} \left(Q_{k_j} \oplus -Q_{k_j} \right), \tag{4.8}$$

where $\lambda_j < 0$ and S is some invertible matrix in Ω_{4n}.

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[7] Included in this thesis as Chapter 2. The specific reference is to Theorem 2.2.4.

[8] Included in this thesis as Chapter 2. The specific reference is to Lemma 2.2.12.

Proof. Let $\tilde{B}$ be an $\tilde{H}$-selfadjoint matrix where both $\tilde{B}$ and $\tilde{H}$ are in Ω_{4n} and $\tilde{B}$ has only negative eigenvalues. Assume that there exists an $\tilde{H}$-selfadjoint mth root $\tilde{A} \in \Omega_{4n}$ of $\tilde{B}$, that is, $\tilde{A}^m = \tilde{B}$. Denote the eigenvalues of $\tilde{B}$ by λ_j, and let μ_j be any mth root of λ_j. Since m is even, μ_j is nonreal. Thus from Theorem 4.2.6, we know that the canonical form of $(\tilde{A}, \tilde{H})$ is (J, Q) where

$$J = \bigoplus_{j=1}^{t} \left(J_{k_j}(\mu_j) \oplus J_{k_j}(\bar{\mu}_j)\right) \oplus \bigoplus_{j=1}^{t} \left(J_{k_j}(\bar{\mu}_j) \oplus J_{k_j}(\mu_j)\right),$$

and

$$Q = \bigoplus_{j=1}^{t} Q_{2k_j} \oplus \bigoplus_{j=1}^{t} Q_{2k_j},$$

for some t. Hence, there exists an invertible matrix $P \in \Omega_{4n}$ such that the equations $P^{-1}\tilde{A}P = J$ and $P^*\tilde{H}P = Q$ hold. Consider

$$P^{-1}\tilde{B}P = (P^{-1}\tilde{A}P)^m = \bigoplus_{j=1}^{t} \left((J_{k_j}(\mu_j))^m \oplus (J_{k_j}(\bar{\mu}_j))^m\right) \oplus \bigoplus_{j=1}^{t} \left((J_{k_j}(\bar{\mu}_j))^m \oplus (J_{k_j}(\mu_j))^m\right),$$

and note that this matrix is $P^*\tilde{H}P$-selfadjoint. Next, by taking

$$T_j = (J_{k_j}(\mu_j))^m \oplus (J_{k_j}(\bar{\mu}_j))^m$$

for $j = 1, \ldots, t$, and applying Lemma 4.3.5 we have that $(T_j \oplus \bar{T}_j,\ Q_{2k_j} \oplus Q_{2k_j})$ is unitarily similar to

$$\left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j),\ Q_{k_j} \oplus -Q_{k_j} \oplus Q_{k_j} \oplus -Q_{k_j}\right),$$

for all $j = 1, \ldots, t$. Therefore, by using the permutation matrix defined in (4.5), we see that the canonical form of $(\tilde{B}, \tilde{H})$ is given by (4.7) and (4.8).

Conversely, let $\tilde{B}$ be $\tilde{H}$-selfadjoint and such that the canonical form of $(\tilde{B}, \tilde{H})$ is given by (4.7) and (4.8), and let m be even. Assume that

$$\tilde{B} = J_n(\lambda) \oplus J_n(\lambda) \oplus J_n(\lambda) \oplus J_n(\lambda) \quad \text{and} \quad \tilde{H} = Q_n \oplus -Q_n \oplus Q_n \oplus -Q_n,$$

where $\lambda < 0$. Then let $J = J_n(\mu) \oplus J_n(\bar{\mu}) \oplus J_n(\bar{\mu}) \oplus J_n(\mu)$ where μ is any mth root of λ. The number μ is nonreal and therefore J is Q-selfadjoint where $Q = Q_{2n} \oplus Q_{2n}$. Note that the matrix J^m has λ on its main diagonal and satisfies the conditions of $T \oplus \bar{T}$ as in Lemma 4.3.5. Thus, it follows that the pair $(J^m,\ Q_{2n} \oplus Q_{2n})$ is unitarily similar to the pair $(\tilde{B}, \tilde{H})$, that is, there exists an invertible matrix $P \in \Omega_{4n}$ such that the equations $P^{-1}J^mP = \tilde{B}$ and $P^*QP = \tilde{H}$ hold. Finally, from Lemma 4.2.5, the matrix $\tilde{A} := P^{-1}JP \in \Omega_{4n}$ is an $\tilde{H}$-selfadjoint mth root of $\tilde{B}$. □

Next, we give the negative eigenvalue case where m is odd. This case is similar to the positive eigenvalue case.

Theorem 4.3.7. *Let $\tilde{H} \in \Omega_{2n}$ be an invertible Hermitian matrix and $\tilde{B} \in \Omega_{2n}$ an $\tilde{H}$-selfadjoint matrix with a spectrum consisting of only negative real numbers. Then, for m odd, there exists an $\tilde{H}$-selfadjoint matrix in Ω_{2n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$.*

Proof. Let $\tilde{B} \in \Omega_{2n}$ be $\tilde{H}$-selfadjoint with only negative real eigenvalues, where $\tilde{H} \in \Omega_{2n}$ is invertible and Hermitian, and let m be odd. Assume that $\tilde{B} = J_n(\lambda) \oplus J_n(\lambda)$ and $\tilde{H} = \varepsilon Q_n \oplus \varepsilon Q_n$, where $\lambda < 0$ and $\varepsilon = \pm 1$. Since m is odd, we can take μ to be the real mth root of λ and let $J = J_n(\mu) \oplus J_n(\mu)$. Then the Jordan normal form of J^m is equal to $\tilde{B}$, and both J and J^m are $\tilde{H}$-selfadjoint. Similarly to Theorem 4.3.3, we can construct an invertible matrix $P \in \Omega_{2n}$ such that the equations

$$P^{-1} J^m P = \tilde{B} \quad \text{and} \quad P^* \tilde{H} P = \tilde{H}$$

hold. Therefore, from Lemma 4.2.5, the matrix $\tilde{A} := P^{-1} J P \in \Omega_{2n}$ is an $\tilde{H}$-selfadjoint mth root of $\tilde{B}$. □

In the case where the matrix $\tilde{B}$ has only the number zero as an eigenvalue, we instantly notice a necessary condition for the existence of an mth root $\tilde{A}$ of $\tilde{B}$. Note that $\tilde{A}$ is not necessarily $\tilde{H}$-selfadjoint. Since each number in the Segre characteristic of $\tilde{A}$ corresponding to the zero eigenvalue occurs twice (see Corollary 4.2.3) and from the way mth roots are formed for nilpotent matrices, see for example [3] and [5][9], the m-tuples in the Segre characteristic (or some reordering thereof) corresponding to the zero eigenvalue of $\tilde{B}$ have to exist in pairs, that is, there are two of each m-tuple. For example, with $m = 4$, if the nonzero part of the Segre characteristic of a nilpotent matrix $\tilde{B} \in \Omega_{20}$ is $(3, 3, 2, 2), (3, 3, 2, 2)$, then the nonzero part of the Segre characteristic of any mth root $\tilde{A} \in \Omega_{20}$ is $(10, 10)$.

Here we need another result from [5][9] which was obtained by applying ω_n to all matrices:

Lemma 4.3.8. *Let A be equal to $J_n(0) \oplus J_n(0)$. Then A^m has Jordan normal form*

$$\bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0) \oplus \bigoplus_{i=1}^{r} J_{a+1}(0) \oplus \bigoplus_{i=1}^{m-r} J_a(0),$$

where $n = am + r$, for $a, r \in \mathbb{Z}$, $0 < r \leq m$.

We now give the result for this last case.

Theorem 4.3.9. *Let $\tilde{H} \in \Omega_{2n}$ be an invertible Hermitian matrix and $\tilde{B} \in \Omega_{2n}$ an $\tilde{H}$-selfadjoint matrix with a spectrum consisting of only the number zero. Then there exists an $\tilde{H}$-selfadjoint matrix in Ω_{2n}, say $\tilde{A}$, such that $\tilde{A}^m = \tilde{B}$ if and only if the following properties hold:*

1. *There exists a reordering of the Segre characteristic of $\tilde{B}$ such that each m-tuple occurs twice and the difference between any two numbers in each m-tuple is at most one.*
2. *By using a reordering satisfying the first property, the canonical form of $(\tilde{B}, \tilde{H})$ is given by $(J_B \oplus J_B,\ H_B \oplus H_B)$ where*

$$J_B = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=r_j+1}^{m} J_{a_j}(0) \right),$$

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[9] Included in this thesis as Chapter 2.

and

$$H_B = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right), \tag{4.9}$$

for some $a_j, r_j \in \mathbb{Z}$ *with* $0 < r_j \leq m$. *The signs are as follows, given in terms of* η_j*, where* η_j *could be either* 1 *or* -1*: If* r_j *(respectively* $m - r_j$*) is even, half of the* $\varepsilon_i^{(j)}$ *for* $i = 1, \ldots, r_j$ *(respectively for* $i = r_j + 1, \ldots, m$*) are equal to* η_j *and the other half are equal to* $-\eta_j$. *If* r_j *(respectively* $m - r_j$*) is odd, there is one more of the* $\varepsilon_i^{(j)}$ *for* $i = 1, \ldots, r_j$ *(respectively for* $i = r_j + 1, \ldots, m$*) equal to* η_j *than to* $-\eta_j$.

Proof. Let $\tilde{B} \in \Omega_{2n}$ be $\tilde{H}$-selfadjoint with only zero in its spectrum, where $\tilde{H} \in \Omega_{2n}$ is invertible and Hermitian. Assume there exists an $\tilde{H}$-selfadjoint mth root $\tilde{A} \in \Omega_{2n}$, that is, $\tilde{A}^m = \tilde{B}$. From Theorem 4.2.6 there exists an invertible matrix $S \in \Omega_{2n}$ such that the canonical form of $(\tilde{A}, \tilde{H})$ is given by

$$S^{-1}\tilde{A}S = \bigoplus_{j=1}^{t} J_{k_j}(0) \oplus \bigoplus_{j=1}^{t} J_{k_j}(0) \quad \text{and} \quad S^{*}\tilde{H}S = \bigoplus_{j=1}^{t} \eta_j Q_{k_j} \oplus \bigoplus_{j=1}^{t} \eta_j Q_{k_j},$$

for some t, k_j and signs $\eta_j = \pm 1$. Consider

$$S^{-1}\tilde{B}S = (S^{-1}\tilde{A}S)^m = \bigoplus_{j=1}^{t} (J_{k_j}(0))^m \oplus \bigoplus_{j=1}^{t} (J_{k_j}(0))^m.$$

Therefore by using Lemma 4.3.8 and the permutation matrix defined in (4.5), the matrix $\tilde{B}$ has Jordan normal form:

$$\bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=1}^{m-r_j} J_{a_j}(0) \right) \oplus \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} J_{a_j+1}(0) \oplus \bigoplus_{i=1}^{m-r_j} J_{a_j}(0) \right), \tag{4.10}$$

where $k_j = a_j m + r_j$, $a_j, r_j \in \mathbb{Z}$ and $0 < r_j \leq m$. Hence, from (4.10), we see that there exists a reordering of the Segre characteristic of $\tilde{B}$ in which each m-tuple occurs twice and where the difference between any two numbers in each m-tuple is at most one.

Since the Jordan normal form of $\tilde{B}$ is given in (4.10), by Theorem 4.2.6 the corresponding matrix in the canonical form is given by $H_B \oplus H_B$ where

$$H_B = \bigoplus_{j=1}^{t} \left(\bigoplus_{i=1}^{r_j} \varepsilon_i^{(j)} Q_{a_j+1} \oplus \bigoplus_{i=r_j+1}^{m} \varepsilon_i^{(j)} Q_{a_j} \right),$$

for $\varepsilon_i^{(j)} = \pm 1$, $i = 1, \ldots, m$, $j = 1, \ldots, t$. From the assumption that an $\tilde{H}$-selfadjoint mth root exists, we know that the two properties given in [5, Theorem 2.5][10] hold. The second property is used to find the signs of H_B. Thus, it follows: if r_j (respectively $m - r_j$) is even, half of the $\varepsilon_i^{(j)}$ for $i = 1, \ldots, r_j$ (respectively for $i = r_j + 1, \ldots, m$) are equal to η_j

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[10] Included in this thesis as Chapter 2. The specific reference is to Theorem 2.2.5.

and the other half are equal to $-\eta_j$. If r_j (respectively $m-r_j$) is odd, there is one more of the $\varepsilon_i^{(j)}$ for $i=1,\dots,r_j$ (respectively for $i=r_j+1,\dots,m$) equal to η_j than to $-\eta_j$.

Conversely, let $\tilde{B}$ be an $\tilde{H}$-selfadjoint matrix and suppose that the two properties in the theorem hold. Assume from the first property that $\tilde{B}=B_1\oplus B_1\in\Omega_{2n}$, where

$$B_1=\bigoplus_{j=1}^{t}\left(\bigoplus_{i=1}^{r_j}J_{a_j+1}(0)\oplus\bigoplus_{i=1}^{m-r_j}J_{a_j}(0)\right),$$

and assume that $\tilde{H}=H_1\oplus H_1$ where $H_1=H_B$ is as in (4.9). Let

$$J=\bigoplus_{j=1}^{t}J_{t_j}(0)\oplus\bigoplus_{j=1}^{t}J_{t_j}(0),$$

where t_j is the sum of the sizes of the blocks in $\tilde{B}$ which correspond to one m-tuple, that is, $t_j=r_j(a_j+1)+(m-r_j)(a_j)=a_jm+r_j$. Thus, by using Lemma 4.3.8 and the permutation matrix defined by (4.5), the Jordan normal form of J^m is equal to $\tilde{B}$. Also, let $Q=\bigoplus_{j=1}^{t}\varepsilon_jQ_{t_j}\oplus\bigoplus_{j=1}^{t}\varepsilon_jQ_{t_j}$ where $\varepsilon_j=\eta_j$ is obtained from the signs of H_B, then J is Q-selfadjoint. According to [5, Theorem 2.5][11], there exists an invertible matrix P_1 such that

$$P_1^{-1}\Big(\bigoplus_{j=1}^{t}J_{t_j}(0)\Big)^m P_1=B_1 \quad\text{and}\quad P_1^*\Big(\bigoplus_{j=1}^{t}\varepsilon_jQ_{t_j}\Big)P_1=H_1.$$

Let $P=P_1\oplus\bar{P}_1$, then P is an invertible matrix in Ω_{2n} and the equations

$$P^{-1}J^mP=\tilde{B}\quad\text{and}\quad P^*QP=\tilde{H}$$

hold. From Lemma 4.2.5, the matrix $\tilde{A}:=P^{-1}JP\in\Omega_{2n}$ is an $\tilde{H}$-selfadjoint mth root of the matrix $\tilde{B}$. □

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[11] Included in this thesis as Chapter 2. The specific reference is to Theorem 2.2.5.

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Chapter 5

Quaternion H-polar decompositions[1]

Abstract. Polar decompositions of quaternion matrices with respect to a given indefinite inner product are studied. Necessary and sufficient conditions for the existence of an H-polar decomposition are found. In the process an equivalent to Witt's theorem on extending H-isometries to H-unitary matrices is given for quaternion matrices.

Keywords. Quaternion matrices, H-polar decompositions, Indefinite inner product, Witt's theorem, Extending isometries, Square roots of matrices.
AMS subject classifications. 15B33, 47B50, 15A23.

5.1 Introduction

Polar decompositions of real and complex matrices with respect to a given indefinite inner product have been studied extensively. Necessary and sufficient conditions for the existence of an H-polar decomposition in the real and complex case are given in [6], whereas in [2] a description of the matrices admitting this decomposition can be found. See also the literature referenced in [2]. Special cases of H-polar decompositions are studied, for example, in [3, 4, 5], and in [10] stability of H-polar decompositions is studied. The study of polar decompositions of quaternion matrices (in the standard inner product space) goes back to 1955, see the paper by Wiegmann [12], and see also Proposition 3.2.5(d) in [11] and [13].

Perusal of these studies suggests the need of results on the extension of isometries via Witt's theorem in the quaternion case, see [5] for the complex case. We also need results on the existence of H-selfadjoint square roots and in [8][2] the general case was studied for quaternion matrices, that is, H-selfadjoint mth roots where m is any positive integer, building on results for the complex case as found in [7][3] and [10].

Let H be an invertible Hermitian matrix with quaternion entries which defines the indefinite inner product $[\cdot,\cdot]$. It will be clear from the context which invertible Hermitian matrix (or indefinite inner product) is meant, when we have more than one inner product

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[2] Included in this thesis as Chapter 4.

[3] Included in this thesis as Chapter 2.

under consideration. For a given square quaternion matrix X, we wish to find necessary and sufficient conditions for the existence of an *H-polar decomposition*, that is, such that $X = UA$ where U is an H-unitary matrix (unitary with respect to $[\cdot,\cdot]$) and A is an H-selfadjoint matrix (selfadjoint with respect to $[\cdot,\cdot]$).

We work mostly with matrices in an indefinite inner product space and which have quaternion entries. Basic theory of quaternion linear algebra can be found in various books and papers, see, for example, the book by Leiba Rodman [11] and [13, 14].

In Section 5.2, we present some preliminary results, definitions and notation which are necessary to follow this chapter. The conditions for the existence of H-selfadjoint square roots of H-selfadjoint quaternion matrices are described in Section 5.3. In Section 5.4, we pave the way for the rest of the chapter with an important result, which is crucial in our proof for polar decompositions. Section 5.5 focuses on the theory of Witt extensions. We give the conditions which prescribe the existence of a Witt extension in the quaternion case as well as the form of such a Witt extension. These will be essential for the main results. We obtain necessary and sufficient conditions for the existence of an H-polar decomposition for a given quaternion matrix in Section 5.6.

5.2 Preliminaries

Denote the skew field of real quaternions by $\mathbb{H}$. Every quaternion $x \in \mathbb{H}$ has the form $x = x_0 + x_1\mathsf{i} + x_2\mathsf{j} + x_3\mathsf{k}$, where $x_i \in \mathbb{R}$ and the elements $\mathsf{i}, \mathsf{j}, \mathsf{k}$ satisfy the following formulas:

$$\mathsf{i}^2 = \mathsf{j}^2 = \mathsf{k}^2 = -1, \quad \mathsf{ij} = -\mathsf{ji} = \mathsf{k}, \quad \mathsf{jk} = -\mathsf{kj} = \mathsf{i}, \quad \mathsf{ki} = -\mathsf{ik} = \mathsf{j}.$$

Let $\bar{x} = x_0 - x_1\mathsf{i} - x_2\mathsf{j} - x_3\mathsf{k}$ denote the conjugate quaternion of x. Denote the set of all vectors with n quaternion entries by $\mathbb{H}^n$. This set $\mathbb{H}^n$ is considered as a right vector space; therefore, scalar multiplication is from the right: $v\alpha$, where $v \in \mathbb{H}^n$, $\alpha \in \mathbb{H}$. Remember that multiplication in $\mathbb{H}$ is not commutative.

Let $\mathbb{H}^{m\times n}$ denote the set of all $m \times n$ matrices in $\mathbb{H}$ and consider it as a left vector space. A matrix $A \in \mathbb{H}^{m\times n}$ can be interpreted as a linear transformation from $\mathbb{H}^n$ to $\mathbb{H}^m$. We will use the linear transformation and the matrix representing the linear transformation interchangeably. Let A be an $m \times n$ quaternion matrix. Then we denote the $m \times n$ matrix in which each entry is the conjugate of the corresponding entry in A by $\bar{A}$. The transpose of $\bar{A}$ is the $n \times m$ matrix denoted by A^*. Note that every $n \times n$ quaternion matrix A can be written as $A = A_1 + \mathsf{j}A_2$, where A_1 and A_2 are $n \times n$ complex matrices.

Definition 5.2.1. A nonzero vector $v \in \mathbb{H}^n$ is called a *(right) eigenvector* of a matrix $A \in \mathbb{H}^{n\times n}$ corresponding to the *(right) eigenvalue* $\lambda \in \mathbb{H}$ if the equality $Av = v\lambda$ holds.

An $n \times n$ quaternion matrix A has left eigenvalues and right eigenvalues, but we only need right eigenvalues and right eigenvectors and therefore omit the word "right".

The *spectrum* of A, denoted by $\sigma(A)$, is the set of all eigenvalues of A and is closed under similarity of quaternions. From [13], we see that an $n\times n$ matrix A has exactly n eigenvalues which are complex numbers with nonnegative imaginary parts and the Jordan normal form of A has precisely these numbers on the diagonal. Let $\mathbb{C}_+ = \{a + \mathsf{i}b \mid a \in \mathbb{R}, b > 0\}$ denote the open upper complex half-plane. The Jordan normal form of a quaternion matrix is a direct sum of Jordan blocks, $J_k(\lambda)$, corresponding to eigenvalue $\lambda \in \mathbb{C}_+$ or $\lambda \in \mathbb{R}$ and of size $k \times k$. We also need the standard involutory permutation (sip) matrix (a $k \times k$ matrix with ones on the main anti-diagonal and zeros elsewhere), and denote it by Q_k.

The null space (or kernel) and the range (or image) of the matrix $A \in \mathbb{H}^{m\times n}$ are as follows:

$$\operatorname{Ker} A = \{x \in \mathbb{H}^n \mid Ax = 0\}; \quad \operatorname{Im} A = \{Ax \mid x \in \mathbb{H}^n\}.$$

An $n \times n$ quaternion matrix H is said to be *Hermitian* if $H^* = H$ and *skew-Hermitian* if $H^* = -H$. The eigenvalues of a Hermitian matrix are real, see Theorem 5.3.6(c) in [11]. Let $\pi(H)$ denote the number of positive eigenvalues of the Hermitian matrix H.

We consider the indefinite inner product $[\,\cdot\,,\cdot\,]$ defined by an invertible Hermitian matrix $H \in \mathbb{H}^{n\times n}$ as follows $[x, y] = \langle Hx, y\rangle = y^*Hx$, for $x, y \in \mathbb{H}^n$, where $\langle\,\cdot\,,\cdot\,\rangle$ denotes the standard inner product. It is important to note that the following is true for all $u, v \in \mathbb{H}^n$ and $\alpha \in \mathbb{H}$:

$$[x, y]^* = [y, x]; \quad [x\alpha, y] = [x, y]\alpha; \quad [x, y\alpha] = \alpha^*[x, y].$$

A subspace W of $\mathbb{H}^n$ is said to be *H-nondegenerate* if $x \in W$ and $[x, y] = 0$ for all $y \in W$ imply that $x = 0$. Otherwise W is H-degenerate.

Let $W^{[\perp]}$ denote the *H-orthogonal companion* of the subspace W of $\mathbb{H}^n$, that is,

$$W^{[\perp]} := \{x \in \mathbb{H}^n \mid [x, y] = 0 \text{ for all } y \in W\}.$$

In terms of the H-orthogonal companion, we have the following result for quaternion subspaces. See Proposition 3.6.4 in [11].

Proposition 5.2.2. *Let W be a subspace of $\mathbb{H}^n$. Then the following are equivalent:*

(i) *W is H-nondegenerate.*

(ii) *$W^{[\perp]}$ is H-nondegenerate.*

(iii) *$W^{[\perp]}$ is a direct complement to W in $\mathbb{H}^n$.*

Definition 5.2.3. Let H_1 and H_2 be the matrices associated with the indefinite inner products $[\,\cdot\,,\cdot\,]_1$ on $\mathbb{H}^n$ and $[\,\cdot\,,\cdot\,]_2$ on $\mathbb{H}^m$, respectively. Let $X : \mathbb{H}^n \to \mathbb{H}^m$ be a linear transformation. Then $X^{[*]} : \mathbb{H}^m \to \mathbb{H}^n$ defined by

$$[X^{[*]}y, x]_1 = [y, Xx]_2,$$

for all $x \in \mathbb{H}^n$, $y \in \mathbb{H}^m$, is called the *H_1-H_2-adjoint* of X.

Note that we can also write $X^{[*]} = H_1^{-1}X^*H_2$. In the case where $n = m$ and $H = H_1 = H_2$, we call $X^{[*]} = H^{-1}X^*H$ the *H-adjoint* of X. A matrix A is said to be *H-selfadjoint* if A coincides with its H-adjoint. An $n \times n$ matrix U is said to be *H-unitary* if $[Ux, Uy] = [x, y]$ for all $x, y \in \mathbb{H}^n$, or equivalently, if $U^*HU = H$. In terms of the H-adjoint, we can also say U is H-unitary if $U^{[*]}U = I$.

With V and W subspaces of $\mathbb{H}^n$, a linear transformation (or its matrix representation) $U : V \to W$ is called an *H-isometry* if $[Ux, Uy] = [x, y]$ for all $x, y \in V$, or equivalently, if $U^*HUx = Hx$ for all $x \in V$.

Every pair (A, H) of quaternion matrices, where A is H-selfadjoint, has a unique canonical form and it is interesting to note that it is identical to the canonical form of complex matrices. This is also given in, for example [1, Theorem 4.1], [9] and [11, Theorem 10.1.1].

Theorem 5.2.4. *Let $H \in \mathbb{H}^{n\times n}$ be an invertible Hermitian matrix and $A \in \mathbb{H}^{n\times n}$ an H-selfadjoint matrix. Then there exists an invertible matrix $S \in \mathbb{H}^{n\times n}$ such that*

$$\begin{aligned} S^{-1}AS &= J_{k_1}(\lambda_1) \oplus \cdots \oplus J_{k_\alpha}(\lambda_\alpha) \\ &\oplus \begin{bmatrix} J_{k_{\alpha+1}}(\lambda_{\alpha+1}) & 0 \\ 0 & J_{k_{\alpha+1}}(\overline{\lambda}_{\alpha+1}) \end{bmatrix} \oplus \cdots \oplus \begin{bmatrix} J_{k_\beta}(\lambda_\beta) & 0 \\ 0 & J_{k_\beta}(\overline{\lambda}_\beta) \end{bmatrix}, \end{aligned} \tag{5.1}$$

where $\lambda_i \in \sigma(A) \cap \mathbb{R}$ for all $i = 1, \ldots, \alpha$, $\lambda_i \in \sigma(A) \cap \mathbb{C}_+$ for all $i = \alpha + 1, \ldots, \beta$, and

$$S^*HS = \eta_1 Q_{k_1} \oplus \cdots \oplus \eta_\alpha Q_{k_\alpha} \oplus Q_{2k_{\alpha+1}} \oplus \cdots \oplus Q_{2k_\beta}, \tag{5.2}$$

where $\eta_i = \pm 1$. The form $(S^{-1}AS,\ S^*HS)$ in (5.1) and (5.2) is uniquely determined by the pair (A, H), up to a permutation of diagonal blocks.

5.3 H-selfadjoint square roots

Necessary and sufficient conditions for the existence of a quaternion H-selfadjoint mth root of a quaternion H-selfadjoint matrix were found in [8][4]. The conditions are stated for matrices in the subalgebra

$$\Omega_{2n} := \left\{ \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix} \mid A_1, A_2 \in \mathbb{C}^{n\times n} \right\}$$

of $\mathbb{C}^{2n\times 2n}$, and $\mathbb{H}^{n\times n}$ is isomorphic to Ω_{2n} by means of the isomorphism ω_n defined by

$$\omega_n(A_1 + \mathsf{j}A_2) = \begin{bmatrix} A_1 & \bar{A}_2 \\ -A_2 & \bar{A}_1 \end{bmatrix}, \quad \text{where } A_1, A_2 \in \mathbb{C}^{n\times n}. \tag{5.3}$$

Then for any $n \times n$ quaternion matrix B we have the following: The canonical form of $(\omega_n(B), \omega_n(H))$ is given by $(J \oplus \bar{J}, Q \oplus Q)$ if and only if the canonical form of (B, H) is given by (J, Q). To see this, apply ω_n to both sides of (5.1) and (5.2), and use the properties $\omega_n(A^*) = (\omega_n(A))^*$ and $\omega_n(A^{-1}) = (\omega_n(A))^{-1}$, where in the latter case, A is invertible.

Now, for a given H-selfadjoint matrix B in $\mathbb{H}^{n\times n}$ we present necessary and sufficient conditions for the existence of an H-selfadjoint square root of B (i.e., $m = 2$ in Theorem 3.2 stated in [8][5]).

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[4] Included in this thesis as Chapter 4.

[5] Included in this thesis as Chapter 4. The specific reference is to Theorem 4.3.2.

Theorem 5.3.1. *Let B and H be $n \times n$ quaternion matrices. Let H be invertible and Hermitian, and let B be H-selfadjoint. Then there exists an H-selfadjoint quaternion matrix, say A, such that $A^2 = B$ if and only if the canonical form of (B, H) has the following properties:*

(i) *The part of the canonical form corresponding to the negative eigenvalues λ_j, say (B_-, H_-), is given by*

$$B_- = \bigoplus_{j=1}^{t_-} \left(J_{k_j}(\lambda_j) \oplus J_{k_j}(\lambda_j)\right), \quad H_- = \bigoplus_{j=1}^{t_-} \left(Q_{k_j} \oplus -Q_{k_j}\right),$$

for some t_-.

(ii) *The part of the canonical form corresponding to the zero eigenvalue, say (B_0, H_0), is given by*

$$B_0 = \bigoplus_{j=1}^{t_0} B^{(j)}, \qquad H_0 = \bigoplus_{j=1}^{t_0} H^{(j)},$$

for some t_0 and where each corresponding pair of matrices $(B^{(j)}, H^{(j)})$ is given by either

$$B^{(j)} = J_{a_j+1}(0) \oplus J_{a_j}(0), \quad H^{(j)} = \eta_j Q_{a_j+1} \oplus \eta_j Q_{a_j},$$

or

$$B^{(j)} = J_{a_j}(0) \oplus J_{a_j}(0), \quad H^{(j)} = Q_{a_j} \oplus -Q_{a_j},$$

where $\eta_j = \pm 1$ and in the former case a_j is allowed to be zero.

5.4 First steps toward H-polar decompositions

Here we present a result for quaternion matrices which is a modification of Lemma 4.1 stated in [6] for complex matrices. We will need this later in the proof of the conditions for an H-polar decomposition and it explains why we need a result on extensions of H-isometries to H-unitary matrices. To this end, a quaternion version of Witt's theorem is proved later.

Lemma 5.4.1. *Let $H_1 \in \mathbb{H}^{n\times n}$ and $H_2 \in \mathbb{H}^{m\times m}$ be the invertible Hermitian matrices which define indefinite inner products $[\cdot,\cdot]_1$ on $\mathbb{H}^n$ and $[\cdot,\cdot]_2$ on $\mathbb{H}^m$, respectively. Let X and Y be linear transformations from $\mathbb{H}^n$ to $\mathbb{H}^m$. Then Y can be written in the form*

$$Y = UX,$$

where U is an injective H_2-isometry from $\operatorname{Im} X$ to $\operatorname{Im} Y$, if and only if both

$$Y^{[*]}Y = X^{[*]}X \tag{5.4}$$

and

$$\operatorname{Ker} X = \operatorname{Ker} Y \tag{5.5}$$

are satisfied.

Before we give the proof, here is an example as an illustration of why injectivity of U is necessary in the lemma.

Example 5.4.2. Let $n = m = 2$ and let X and Y be given as

$$X = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Let $H_1 = H_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ be the matrix defining the indefinite inner product on $\mathbb{H}^2$. Then $\operatorname{Im} X = \operatorname{span}\left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix} \right\}$ and $\operatorname{Im} Y = \left\{ \begin{bmatrix} 0 \\ 0 \end{bmatrix} \right\}$. Now suppose $U : \operatorname{Im} X \to \operatorname{Im} Y$ is a linear transformation such that $Y = UX$. For any $\alpha, \beta \in \mathbb{H}$, we have

$$\left[U \begin{bmatrix} \alpha \\ 0 \end{bmatrix}, U \begin{bmatrix} \beta \\ 0 \end{bmatrix} \right]_2 = [0, 0]_2 = 0$$

and

$$\left[\begin{bmatrix} \alpha \\ 0 \end{bmatrix}, \begin{bmatrix} \beta \\ 0 \end{bmatrix} \right]_2 = \left\langle \begin{bmatrix} 0 \\ \alpha \end{bmatrix}, \begin{bmatrix} \beta \\ 0 \end{bmatrix} \right\rangle = 0.$$

Therefore, U is an H_2-isometry, but note that $Ux = Uy = 0$ for all $x, y \in \operatorname{Im} X$ and it does not imply that $x = y$, so U is not injective. Now,

$$X^{[*]}X = H_1^{-1} X^* H_2 X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

and $Y^{[*]}Y = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} = X^{[*]}X$. However, we have

$$\operatorname{Ker} Y = \mathbb{H}^2 \quad \text{and} \quad \operatorname{Ker} X = \operatorname{span}\left\{ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\},$$

thus the null spaces do not coincide. □

Now for the proof of Lemma 5.4.1. The proof is essentially the same as in [6], but a change to right scalar multiplication was needed.

Proof. Suppose that $Y = UX$, where U is an injective H_2-isometry from $\operatorname{Im} X$ to $\operatorname{Im} Y$. Then

$$Y^{[*]}Y = X^{[*]}U^{[*]}UX = X^{[*]}X.$$

Since U is injective, we have $\operatorname{Ker} Y = \operatorname{Ker} UX = \operatorname{Ker} X$. Therefore, both (5.4) and (5.5) hold.

Conversely, assume that both (5.4) and (5.5) hold. We want to find an injective H_2-isometry between $\operatorname{Im} X$ and $\operatorname{Im} Y$. Let the dimension of $\operatorname{Im} X$ be p and let $\{f_1, \ldots, f_p\}$ be a basis of $\operatorname{Im} X \subseteq \mathbb{H}^m$. Now let $\{e_1, \ldots, e_p\}$ be vectors in $\mathbb{H}^n$ such that

$$Xe_i = f_i, \quad i = 1, 2, \ldots, p, \tag{5.6}$$

and let g_i be the image of e_i under Y, that is,

$$g_i = Ye_i, \quad i = 1, 2, \ldots, p. \tag{5.7}$$

We prove that the set $\{g_1, \ldots, g_p\}$ is a basis of $\operatorname{Im} Y$. If for some quaternion scalars γ_i we have

$$\sum_{i=1}^{p} g_i \gamma_i = 0,$$

then it follows from (5.7) and (5.5) that $\sum_{i=1}^{p} e_i\gamma_i \in \operatorname{Ker} Y = \operatorname{Ker} X$. This implies that

$$\sum_{i=1}^{p} f_i\gamma_i = X \sum_{i=1}^{p} e_i\gamma_i = 0,$$

but since $\{f_1, \ldots, f_p\}$ is a basis, $\gamma_1 = \gamma_2 = \cdots = \gamma_p = 0$. Therefore, the vectors $\{g_1, \ldots, g_p\}$ are linearly independent. From (5.5) and the Rank Theorem (see Proposition 3.2.5(e) in [11]), we have that $\dim \operatorname{Im} Y = p$ and hence the p vectors in (5.7) form a basis of $\operatorname{Im} Y$. Finally, define the linear map $U' : \operatorname{Im} X \to \operatorname{Im} Y$ by

$$U'f_i = g_i, \quad i = 1, 2, \ldots, p.$$

Let $a = \sum_{i=1}^{p} f_i\alpha_i$ and $b = \sum_{i=1}^{p} f_i\beta_i$ be arbitrary vectors in $\operatorname{Im} X$, $\alpha_i, \beta_i \in \mathbb{H}$. Then using (5.4), (5.6), and (5.7), it can be shown that $[U'a, U'b]_2 = [a, b]_2$:

$$\begin{aligned}
[U'a, U'b]_2 &= [U'(f_1\alpha_1 + \cdots + f_p\alpha_p), U'(f_1\beta_1 + \cdots + f_p\beta_p)]_2 \\
&= [g_1\alpha_1 + \cdots + g_p\alpha_p, g_1\beta_1 + \cdots + g_p\beta_p]_2 \\
&= [Ye_1\alpha_1 + \cdots + Ye_p\alpha_p, Ye_1\beta_1 + \cdots + Ye_p\beta_p]_2 \\
&= [Y(e_1\alpha_1 + \cdots + e_p\alpha_p), Y(e_1\beta_1 + \cdots + e_p\beta_p)]_2 \\
&= [Y^{[*]}Y(e_1\alpha_1 + \cdots + e_p\alpha_p), (e_1\beta_1 + \cdots + e_p\beta_p)]_1 \\
&= [X^{[*]}X(e_1\alpha_1 + \cdots + e_p\alpha_p), (e_1\beta_1 + \cdots + e_p\beta_p)]_1 \\
&= [Xe_1\alpha_1 + \cdots + Xe_p\alpha_p, Xe_1\beta_1 + \cdots + Xe_p\beta_p]_2 \\
&= [a, b]_2
\end{aligned}$$

and thus U' is an H_2-isometry. Assume $U'a = 0$, then $\sum_{i=1}^{p} g_i\alpha_i = 0$ but the vectors $\{g_1, \ldots, g_p\}$ are linearly independent and therefore $a = 0$. This implies that U' is injective and we conclude the proof. ☐

5.5 Witt's theorem

Witt's theorem is known for vector spaces over the real and complex numbers, and gives conditions for the extension of isometries between subspaces of $\mathbb{F}^n$ (where $\mathbb{F}$ is the field of real or complex numbers) to the whole of $\mathbb{F}^n$. Witt's theorem is an indispensable tool in the study of H-polar decompositions. We extend Witt's theorem to the quaternion case by supplying a proof that is essentially the same as the proof of Theorem 2.1 in [5].

Theorem 5.5.1. *Let* $H_1, H_2 \in \mathbb{H}^{n\times n}$ *be invertible Hermitian matrices which define two inner products* $[\,\cdot\,,\cdot\,]_1$ *and* $[\,\cdot\,,\cdot\,]_2$ *on* $\mathbb{H}^n$*, respectively. Assume that* $\pi(H_1) = \pi(H_2)$*. Let* $U_0 : V_1 \to V_2$ *be a nonsingular linear transformation, where* V_1 *and* V_2 *are subspaces in* $\mathbb{H}^n$*, such that*

$$[U_0x, U_0y]_2 = [x, y]_1 \quad \text{for every} \quad x, y \in V_1. \tag{5.8}$$

Then there exists a linear transformation $U : \mathbb{H}^n \to \mathbb{H}^n$ *such that*

$$[Ux, Uy]_2 = [x, y]_1 \quad \text{for every} \quad x, y \in \mathbb{H}^n \tag{5.9}$$

and

$$Ux = U_0x \quad \text{for every} \quad x \in V_1. \tag{5.10}$$

Any linear transformation U with the property (5.9) is called H_1-H_2-*unitary* and any H_1-H_2-unitary linear transformation that also satisfies (5.10) is called a *Witt extension* of U_0.

Proof. Let m be the dimension of V_1 and let $\{e_1, \ldots, e_m\}$ be a basis of $V_1 \subseteq \mathbb{H}^n$ such that

$$[e_i, e_j]_1 = \begin{cases} 1 & \text{if } \ i = j = m_0 + 1, m_0 + 2, \ldots, m_0 + m_+, \\ -1 & \text{if } \ i = j = m_0 + m_+ + 1, m_0 + m_+ + 2, \ldots, m, \\ 0 & \text{otherwise}, \end{cases}$$

where $m_0 + m_+ + m_- = m$. Thus, the Hermitian matrix describing the restriction of the inner product $[\,\cdot\,,\cdot\,]_1$ to V_1 has m_+ positive eigenvalues and m_- negative eigenvalues and the multiplicity of zero is m_0.

The strategy that we follow is to construct a basis for $\mathbb{H}^n$ using the basis for V_1 and we start by forming H_1-nondegenerate subspaces where each contains one of the first m_0 basis vectors. Define a functional $\alpha_i : \mathbb{H}^n \to \mathbb{H}$ for every $i = 1, 2, \ldots, m$ as follows:

$$\alpha_i(x) = [x, e_i]_1, \quad i = 1, 2, \ldots, m.$$

Since $\alpha_1, \ldots, \alpha_m$ are linearly independent, there exist vectors $\tilde{e}_i \in \mathbb{H}^n$ such that $\alpha_i(\tilde{e}_j) = \delta_{ij}$, where $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$, that is, $[\tilde{e}_j, e_i]_1 = \delta_{ij}$ for all $i = 1, 2, \ldots, m$. Then let

$$W_k = \operatorname{span}\{e_k, \tilde{e}_k\}, \quad k = 1, 2, \ldots, m_0$$

and since $[e_k, e_k]_1 = 0$ and $[\tilde{e}_k, e_k]_1 = 1$, each W_k is H_1-nondegenerate. Note that for $\beta_k = -\frac{1}{2}[\tilde{e}_k, \tilde{e}_k]_1$, we have

$$\begin{aligned} [\tilde{e}_k + e_k\beta_k, \tilde{e}_k + e_k\beta_k]_1 &= [\tilde{e}_k, \tilde{e}_k]_1 + [e_k\beta_k, e_k\beta_k]_1 + [\tilde{e}_k, e_k\beta_k]_1 + [e_k\beta_k, \tilde{e}_k]_1 \\ &= [\tilde{e}_k, \tilde{e}_k]_1 + \beta_k^*[e_k, e_k]_1\beta_k + \beta_k^*[\tilde{e}_k, e_k]_1 + [e_k, \tilde{e}_k]_1\beta_k \\ &= [\tilde{e}_k, \tilde{e}_k]_1 - \frac{1}{2}[\tilde{e}_k, \tilde{e}_k]_1 - \frac{1}{2}[\tilde{e}_k, \tilde{e}_k]_1 = 0, \end{aligned}$$

and

$$[e_k, \tilde{e}_k + e_k\beta_k]_1 = [e_k, \tilde{e}_k]_1 + \beta_k^*[e_k, e_k]_1 = [e_k, \tilde{e}_k]_1.$$

Therefore, we can always replace the vector $\tilde{e}_k$ by $\tilde{e}_k + e_k\left(-\frac{1}{2}[\tilde{e}_k, \tilde{e}_k]_1\right)$ and thus without loss of generality we can assume that $[\tilde{e}_k, \tilde{e}_k]_1 = 0$ for $k = 1, 2, \ldots, m_0$. Now, let

$$e'_k = (e_k - \tilde{e}_k)\frac{1}{\sqrt{2}}, \qquad e''_k = (e_k + \tilde{e}_k)\frac{1}{\sqrt{2}}.$$

Simple calculations analogous to those above give the following:

$$[e'_k, e'_k]_1 = -1, \quad [e''_k, e''_k]_1 = 1 \quad \text{and} \quad [e'_k, e''_k]_1 = 0.$$

It follows that the subspace $W = W_1 + \cdots + W_{m_0} + \operatorname{span}\{e_j\}_{i=m_0+1,\ldots,m}$ is H_1-nondegenerate and thus by Proposition 5.2.2 the H_1-orthogonal companion $W^{[\perp]}$ of W is H_1-nondegenerate and $W^{[\perp]}$ is a direct complement to W in $\mathbb{H}^n$. Therefore, we can append the vectors e_s for $s = 2m_0 + m_+ + m_- + 1, 2m_0 + m_+ + m_- + 2, \ldots, n$ to the set

$$\{e'_1, \ldots, e'_{m_0}, e''_1, \ldots, e''_{m_0}, e_{m_0+1}, e_{m_0+2}, \ldots, e_m\}$$

of $2m_0 + m_+ + m_-$ vectors such that the resulting ordered set $\{g_1, \ldots, g_n\}$ will be a basis in $\mathbb{H}^n$ with the property

$$[g_i, g_j]_1 = \varepsilon_i \delta_{ij}, \quad \text{for } i, j = 1, 2, \ldots, n, \text{ where } \varepsilon_i = \pm 1.$$

As a last step before we can define the extension, we look at the subspace V_2. Let $f_i = U_0 e_i$ for $i = 1, 2, \ldots, m$. We introduce vectors f'_k and f''_k (for $k = 1, 2, \ldots, m$) and vectors f_s (for $s = 2m_0 + m_+ + m_- + 1, 2m_0 + m_+ + m_- + 2, \ldots, n$) in the same way we introduced the vectors e'_k, e''_k, and e_s but using $[\cdot,\cdot]_2$ instead of $[\cdot,\cdot]_1$. Then this will result in a basis $\{h_1, \ldots, h_n\}$ of $\mathbb{H}^n$. The hypotheses $\pi(H_1) = \pi(H_2)$ and (5.8) in the theorem statement ensure that $[h_i, h_j]_2 = [g_i, g_j]_1$ for all $i, j = 1, \ldots, n$.

Finally, we define the $n \times n$ matrix U by the equalities:

$$\begin{array}{ll} Ue'_k = f'_k, & \text{for } k = 1, \ldots, m_0, \\ Ue''_k = f''_k, & \text{for } k = 1, \ldots, m_0, \\ Ue_j = f_j, & \text{for } j = m_0 + 1, \ldots, m, \\ Ue_s = f_s, & \text{for } s = 2m_0 + m_+ + m_- + 1, \ldots, n. \end{array}$$

From the construction above, it is easy to see that the matrix U satisfies both (5.9) and (5.10) and is therefore a Witt extension of U_0. □

We next include an extended Witt's theorem which gives a description of any Witt extension of a given U_0. The proof in the quaternion case is once again essentially the same as the proof of Theorem 2.3 in [5].

Firstly, we mention the following: using the same notation (and vectors) as in the proof of Theorem 5.5.1, let

$$\mathcal{E} = \{e_1, \ldots, e_{m_0}, e_{m_0+1}, \ldots, e_m, \tilde{e}_1, \ldots, \tilde{e}_{m_0}, e_{2m_0+m_++m_-+1}, \ldots, e_n\}, \tag{5.11}$$

$$\mathcal{F} = \{Ue_1, \ldots, Ue_m, U\tilde{e}_1, \ldots, U\tilde{e}_{m_0}, Ue_{2m_0+m_++m_-+1}, \ldots, Ue_n\}. \tag{5.12}$$

Note that the subspaces V_1 and V_2 are spanned by the first m vectors of the bases of $\mathcal{E}$ and $\mathcal{F}$, respectively. The Gramian matrix of the basis $\mathcal{E}$ with respect to $[\cdot,\cdot]_1$ (and of the basis $\mathcal{F}$ with respect to $[\cdot,\cdot]_2$) is equal to

$$\begin{bmatrix} 0 & 0 & I_{m_0} & 0 \\ 0 & J_1 & 0 & 0 \\ I_{m_0} & 0 & 0 & 0 \\ 0 & 0 & 0 & J_2 \end{bmatrix}, \tag{5.13}$$

where J_1 and J_2 are both diagonal matrices with $+1$ and -1 on its diagonal. The first m_+ diagonal entries of J_1 are $+1$ and the remaining m_- diagonal entries are -1. The matrix J_2 is the Gramian matrix of the last $n-m-m_0$ vectors in (5.11) and we assume without loss of generality that it has said form.

Theorem 5.5.2. *Let $\tilde{U}$ be a Witt extension of the $n \times n$ matrix U_0 as in Theorem 5.5.1. Then there exists a J_2-unitary matrix P_1 (of size $n-m-m_0$), an $(n-m-m_0) \times m_0$ matrix P_2, and a skew-Hermitian $m_0 \times m_0$ matrix P_3, such that the matrix of $\tilde{U}$ has the form*

$$\tilde{U} = \begin{bmatrix} I_{m_0} & 0 & -\frac{1}{2}P_2^* J_2 P_2 + P_3 & -P_2^* J_2 P_1 \\ 0 & I_{m-m_0} & 0 & 0 \\ 0 & 0 & I_{m_0} & 0 \\ 0 & 0 & P_2 & P_1 \end{bmatrix}. \tag{5.14}$$

Here $m = \dim V_1$ and m_0 is the algebraic multiplicity of the zero eigenvalue of the Gramian matrix of any basis in V_1 with respect to $[\cdot,\cdot]_1$.

Conversely, if P_1 is an arbitrary J_2-unitary matrix, P_2 is an arbitrary $(n-m-m_0)\times m_0$ matrix, and P_3 is an arbitrary skew-Hermitian $m_0 \times m_0$ matrix, then the matrix $\tilde{U}$ defined by (5.14) is a Witt extension of U_0.

Proof. To ensure that $\tilde{U}x = U_0 x$ for all $x \in V_1$, any extension $\tilde{U}$ of U_0 in the bases (5.11) and (5.12) has the form

$$\tilde{U} = \begin{bmatrix} I & 0 & A_1 & A_2 \\ 0 & I & A_3 & A_4 \\ 0 & 0 & A_5 & A_6 \\ 0 & 0 & A_7 & A_8 \end{bmatrix}, \tag{5.15}$$

for some matrices A_i with sizes the same as the corresponding blocks in (5.13). The key to proving the theorem lies in the following: the matrix (5.15) is H_1-H_2-unitary if and only if $H_1^{-1}\tilde{U}^* H_2 \tilde{U} = I$. Using (5.13) and (5.15), a simple computation shows that $H_1^{-1}\tilde{U}^* H_2 \tilde{U} = I$ holds if and only if

$$\begin{bmatrix} A_5^* & A_3^* J_1 & u_{13} & u_{14} \\ 0 & I & A_3 & A_4 \\ 0 & 0 & A_5 & A_6 \\ J_2 A_6^* & J_2 A_4^* J_1 & u_{43} & u_{44} \end{bmatrix} = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}, \tag{5.16}$$

where

$$\begin{aligned} u_{13} &= A_5^*A_1 + A_3^*J_1A_3 + A_1^*A_5 + A_7^*J_2A_7, \\ u_{14} &= A_5^*A_2 + A_3^*J_1A_4 + A_1^*A_6 + A_7^*J_2A_8, \\ u_{43} &= J_2A_6^*A_1 + J_2A_4^*J_1A_3 + J_2A_2^*A_5 + J_2A_8^*J_2A_7, \\ u_{44} &= J_2A_6^*A_2 + J_2A_4^*J_1A_4 + J_2A_2^*A_6 + J_2A_8^*J_2A_8. \end{aligned}$$

By equating the corresponding blocks in (5.16), we obtain the following:

$$A_5 = I,\ A_3 = A_4 = A_6 = 0,\ A_2 = -A_7^*J_2A_8,\ A_8^*J_2A_8 = J_2 \text{ and } A_1 + A_1^* = -A_7^*J_2A_7. \tag{5.17}$$

When we write $A_1 = \frac{1}{2}(A_1 + A_1^*) + \frac{1}{2}(A_1 - A_1^*)$, where the first term is Hermitian and the second is skew-Hermitian, we can use the last equality in (5.17) to find an expression for A_1. Then by taking $P_1 = A_8$, $P_2 = A_7$ and $P_3 = \frac{1}{2}(A_1 - A_1^*)$, the matrix (5.14) in the theorem statement is derived and the proof is complete. □

5.6 *H*-polar decompositions

Finally, we are ready to give necessary and sufficient conditions for the existence of an H-polar decomposition of a given quaternion matrix.

Theorem 5.6.1. *Let H be an invertible Hermitian matrix in $\mathbb{H}^{n\times n}$. Then a given matrix $X \in \mathbb{H}^{n\times n}$ admits an H-polar decomposition, say $X = UA$ for an H-selfadjoint A and an H-unitary U, if and only if there exists an H-selfadjoint square root A of $X^{[*]}X$ with* $\operatorname{Ker} X = \operatorname{Ker} A$.

Proof. Assume that there exists an $n \times n$ H-unitary matrix U and an $n \times n$ H-selfadjoint matrix A such that $X = UA$. Then

$$X^{[*]}X = (UA)^{[*]}UA = A^{[*]}U^{[*]}UA = AA = A^2,$$

that is, A is an H-selfadjoint square root of $X^{[*]}X$. Also note that U is invertible and therefore,

$$\operatorname{Ker} X = \operatorname{Ker} UA = \operatorname{Ker} A.$$

Conversely, suppose that there exists an H-selfadjoint square root A of $X^{[*]}X$, that is, $X^{[*]}X = A^2$, such that $\operatorname{Ker} X = \operatorname{Ker} A$. Since A is H-selfadjoint, we can write $X^{[*]}X = A^{[*]}A$. Then, by Lemma 5.4.1, there exists an injective H-isometry U_0 from $\operatorname{Im} A$ to $\operatorname{Im} X$ such that $X = U_0A$. Note that the conditions in Theorem 5.5.1 are satisfied where $V_1 = \operatorname{Im} A$ and $V_2 = \operatorname{Im} X$, and therefore we can form a Witt extension of the H-isometry to the whole space $\mathbb{H}^n$. That is, there exists a matrix $U \in \mathbb{H}^{n\times n}$ such that $[Ux, Uy] = [x, y]$ for all $x, y \in \mathbb{H}^n$ and $Ux = U_0x$ for all $x \in \operatorname{Im} A$. Hence, U is H-unitary and $X = U_0A = UA$ which means that X admits an H-polar decomposition. □

Using Theorem 5.3.1, we can rewrite the criterion for the existence of an H-polar decomposition as follows (similarly to Theorem 4.4 in [2]).

Theorem 5.6.2. *Let $H \in \mathbb{H}^{n\times n}$ be an invertible Hermitian matrix. Then a given $X \in \mathbb{H}^{n\times n}$ admits an H-polar decomposition if and only if all of the following conditions are satisfied.*

(i) *Each block in the canonical form of $(X^{[*]}X, H)$ that corresponds to a negative eigenvalue λ_i of $X^{[*]}X$ is of the form*

$$(J_{k_i}(\lambda_i) \oplus J_{k_i}(\lambda_i),\, Q_{k_i} \oplus -Q_{k_i})\,.$$

(ii) *Each block in the canonical form of $(X^{[*]}X, H)$ that corresponds to the zero eigenvalue of $X^{[*]}X$ is either of the form*

$$(B_i, H_i) = (J_{k_i+1}(0) \oplus J_{k_i}(0),\, \eta_i Q_{k_i+1} \oplus \eta_i Q_{k_i})\,,$$

or of the form

$$(B_i, H_i) = (J_{k_i}(0) \oplus J_{k_i}(0),\, Q_{k_i} \oplus -Q_{k_i})\,,$$

where $\eta_i = \pm 1$ and where k_i is allowed to be zero in the former case. We use B_0 for the $k_0 \times k_0$ zero matrix, that is, for all the single blocks $J_1(0)$, and H_0 for the corresponding $k_0 \times k_0$ diagonal matrix with $+1$ and -1 on the diagonal.

(iii) *Let ℓ_i denote the size of a block B_i. There is a choice of basis $\{e_{i,j}\}_{i=0}^{m}{}_{j=1}^{\ell_i}$ in $\mathbb{H}^n$ which produces the canonical form in the second assertion and*

$$\begin{aligned}\operatorname{Ker} X = {} & \operatorname{span}\{e_{i,1} + e_{i,k_1+1} \mid \ell_i = 2k_i, i = 1, \ldots, m\} \\ & \oplus \operatorname{span}\{e_{i,1} \mid \ell_i = 2k_i - 1, i = 1, \ldots, m\} \oplus \operatorname{span}\{e_{0,j}\}_{j=1}^{k_0}.\end{aligned} \tag{5.18}$$

Proof. Let $X \in \mathbb{H}^{n\times n}$ be given and suppose that assertions (i) to (iii) in the theorem statement hold. We want to prove that there exists an H-selfadjoint square root A of $X^{[*]}X$ for which $\operatorname{Ker} X = \operatorname{Ker} A$ holds. Then by Theorem 5.6.1, the matrix X admits an H-polar decomposition and the proof is complete. Since (i) and (ii) are satisfied, Theorem 5.3.1 implies that $X^{[*]}X$ has an H-selfadjoint square root. The strategy that we now follow is to construct for each block B_i as in (ii) of the theorem statement, an H_i-selfadjoint matrix A_i such that $A_i^2 = B_i$ and $\operatorname{Ker} A_i = \operatorname{Ker} X \cap \operatorname{span}\{e_{i,j}\}_{j=1}^{\ell_i}$. Firstly, let B_i be of even size, say $\ell_i = 2k_i$, $k_i \geq 1$. As in the proof of Theorem 4.4 in [2], let S_i be the matrix with columns

$$\begin{gathered}(e_{i,1} + e_{i,k_i+1})\tfrac{1}{\sqrt{2}},\ (e_{i,1} - e_{i,k_i+1})\tfrac{1}{\sqrt{2}},\ (e_{i,2} + e_{i,k_i+2})\tfrac{1}{\sqrt{2}},\ (e_{i,2} - e_{i,k_i+2})\tfrac{1}{\sqrt{2}}, \ldots, \\ (e_{i,k_i} + e_{i,2k_i})\tfrac{1}{\sqrt{2}},\ (e_{i,k_i} - e_{i,2k_i})\tfrac{1}{\sqrt{2}}.\end{gathered}$$

Then $A_i = S_i J_{2k_i}(0) S_i^{-1}$ is an H_i-selfadjoint square root of B_i and

$$\operatorname{Ker} A_i = \operatorname{span}\{e_{i,1} + e_{i,k_i+1}\} = \operatorname{Ker} X \cap \operatorname{span}\{e_{i,j}\}_{j=1}^{\ell_i}.$$

Secondly, let B_i be of odd size, say $\ell_i = 2k_i - 1$, $k_i \geq 1$. Again, as in [2], let S_i be the matrix with columns

$$e_{i,1},\ e_{i,k_i+1},\ e_{i,2},\ e_{i,k_i+2}, \ldots,\ e_{i,k_i-1},\ e_{i,2k_i-1},\ e_{i,k_i}.$$

Then $A_i = S_i J_{2k_i-1}(0) S_i^{-1}$ is an H_i-selfadjoint square root of B_i and

$$\operatorname{Ker} A_i = \operatorname{span}\{e_{i,1}\} = \operatorname{Ker} X \cap \operatorname{span}\{e_{i,j}\}_{j=1}^{\ell_i}.$$

Hence, if A is the H-selfadjoint square root of B consisting of a direct sum of all the A_i's, then we have that $\operatorname{Ker} X = \operatorname{Ker} A$.

Conversely, suppose that $X \in \mathbb{H}^{n\times n}$ admits an H-polar decomposition, say $X = UA$, where $U \in \mathbb{H}^{n\times n}$ is H-unitary and $A \in \mathbb{H}^{n\times n}$ is H-selfadjoint. By Theorem 5.6.1, the H-selfadjoint A is a square root of the H-selfadjoint matrix $X^{[*]}X$ for which $\operatorname{Ker} X = \operatorname{Ker} A$ holds. Since $X^{[*]}X$ has an H-selfadjoint square root, the canonical form of the pair $(X^{[*]}X, H)$ satisfies the conditions in Theorem 5.3.1. Thus, assertions (i) and (ii) hold and there exists a choice of basis $\{e_{i,j}\}_{i=0}^{m}{}_{j=1}^{\ell_i}$ in $\mathbb{H}^n$ which provides the canonical form as given in (ii). Using this basis and a construction for A, as was done above, one can easily see that $\operatorname{Ker} A$ is equal to the right-hand side of (5.18) and since $\operatorname{Ker} X = \operatorname{Ker} A$, we conclude the proof. □

Remark 5.6.3. Since there exists an isomorphism between $\mathbb{H}^{n\times n}$ and Ω_{2n}, all of the results and specifically the conditions for the existence of an H-polar decomposition are also true in Ω_{2n}. In a previous paper, [8][6], proofs were given for matrices in Ω_{2n} as well as an explanation that they are also true for matrices in $\mathbb{H}^{n\times n}$ via the isomorphism ω_n as defined in (5.3). Here, however, we took a direct approach and proved the results for quaternion matrices.

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[6] Included in this thesis as Chapter 4.

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