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Dedicated to the memory of Gene Golub

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DECOMPOSITIONS OF QUATERNIONS AND THEIR MATRIX EQUIVALENTS

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Abstract. Since quaternions have isomorphic representations in matrix form we investigate various well known matrix decompositions for quaternions.

Key words. Decompositions of quaternions, Schur, polar, SVD, Jordan, QR, LU.

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1. Introduction. We will study various decompositions of quaternions where we will employ the isomorphic matrix images of quaternions. The matrix decompositions allow in many cases analogue decompositions of the underlying quaternion.

Let us denote the skew field of quaternions by $\mathbb{H}$. It is well known that quaternions have an isomorphic representation either by certain complex (2×2)-matrices or by certain real (4×4)-matrices. Let $a := (a_1, a_2, a_3, a_4) \in \mathbb{H}$. Then the two isomorphisms $\jmath : \mathbb{H} \to \mathbb{C}^{2\times 2}$, $\imath_1 : \mathbb{H} \to \mathbb{R}^{4\times 4}$ are defined as follows:

$$\jmath(a) := \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \in \mathbb{C}^{2\times 2}, \quad \alpha := a_1 + a_2\mathbf{i},\ \beta := a_3 + a_4\mathbf{i}, \tag{1.1}$$

$$\imath_1(a) := \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ a_2 & a_1 & -a_4 & a_3 \\ a_3 & a_4 & a_1 & -a_2 \\ a_4 & -a_3 & a_2 & a_1 \end{pmatrix} \in \mathbb{R}^{4\times 4}. \tag{1.2}$$

There is another very similar, but nevertheless different mapping, $\imath_2 : \mathbb{H} \to \mathbb{R}^{4\times 4}$, the meaning of which will be explained immediately:

$$\imath_2(a) := \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ a_2 & a_1 & a_4 & -a_3 \\ a_3 & -a_4 & a_1 & a_2 \\ a_4 & a_3 & -a_2 & a_1 \end{pmatrix} \in \mathbb{R}^{4\times 4}. \tag{1.3}$$

In the first equation (1.1) the overlined quantities $\overline{\alpha}, \overline{\beta}$ denote the complex conjugates of the non overlined quantities α, β, respectively. Let $b \in \mathbb{H}$ be another quaternion. Then, the isomorphisms imply $\jmath(ab) = \jmath(a)\jmath(b)$, $\imath_1(ab) = \imath_1(a)\imath_1(b)$. The third map, $\imath_2$, has the interesting property that it reverses the order of the multiplication:

$$\imath_2(ab) = \imath_2(b)\imath_2(a) \text{ for all } a, b \in \mathbb{H}, \quad \imath_1(a)\imath_2(b) = \imath_2(b)\imath_1(a) \text{ for all } a, b \in \mathbb{H}. \tag{1.4}$$

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The mapping $\imath_2$ plays a central role in the investigations of linear maps $\mathbb{H} \to \mathbb{H}$. There is a formal similarity to the Kronecker product of two arbitrary matrices. See [9, Janovská & Opfer, 2007] for the mentioned linear maps and [4, Horn & Johnson, 1991, Lemma 4.3.1] for the Kronecker product.

Definition 1.1. A complex (2×2)-matrix of the form introduced in (1.1) will be called a *complex q-matrix*. A real (4×4)-matrix of the form introduced in (1.2) will be called a *real q-matrix*. A real (4×4)-matrix of the form introduced in (1.3) will be called a *real pseudo q-matrix*. The set of all complex q-matrices will be denoted by $\mathbb{H}_{\mathbb{C}}$. The set of all real q-matrices will be denoted by $\mathbb{H}_{\mathbb{R}}$. The set of all real pseudo q-matrices will be denoted by $\mathbb{H}_{\mathbb{P}}$.

We introduce some common notation. Let $\mathbf{C}$ be a matrix of any size with real or complex entries. By $\mathbf{D} := \mathbf{C}^{\mathrm{T}}$ we denote the *transposed matrix* of $\mathbf{C}$, where rows and columns are interchanged. By $\mathbf{E} := \overline{\mathbf{C}}$ we denote the *conjugate matrix* of $\mathbf{C}$ where all entries of $\mathbf{C}$ are changed to their complex conjugates. Finally, $\mathbf{C}^* := (\overline{\mathbf{C}})^{\mathrm{T}}$. Let $a := (a_1, a_2, a_3, a_4) \in \mathbb{H}$. The first component, a_1, is called the *real part* of a, denoted by $\Re a$. The quaternion $a_v := (0, a_2, a_3, a_4)$ will be called *vector part* of a.

From the above representations it is clear how to recover a quaternion from the corresponding matrix. Thus, it is also possible to introduce inverse mappings

$$\jmath^{-1} : \mathbb{H}_{\mathbb{C}} \to \mathbb{H}, \quad \imath_1^{-1} : \mathbb{H}_{\mathbb{R}} \to \mathbb{H}, \quad \imath_2^{-1} : \mathbb{H}_{\mathbb{P}} \to \mathbb{H},$$

where $\jmath^{-1}$, $\imath_1^{-1}$ as well define isomorphisms. If we define a new algebra $\tilde{\mathbb{H}}$ where a new multiplication, denoted by $\star$ is introduced by $a \star b := ba$, then $\imath_2$ is also an isomorphism between $\tilde{\mathbb{H}}$ and $\mathbb{H}_{\mathbb{P}}$. This particularly implies that $\imath_2(ab) = \imath_2(b)\imath_2(a) \in \mathbb{H}_{\mathbb{P}}$ and $\imath_2(a^{-1}) = \imath_2(a)^{-1} = \imath_2(a)^{\mathrm{T}}/|a|^2 \in \mathbb{H}_{\mathbb{P}}$ for all $a \in \mathbb{H}\backslash\{0\}$. Because of these isomorphisms it is possible to associate notions known from matrix theory with quaternions. Simple examples are:

$$\det(a) := \det(\jmath(a)) = |a|^2, \quad \det(\imath_1(a)) = \det(\imath_2(a)) = |a|^4, \tag{1.5}$$

$$\mathrm{tr}(a) := \mathrm{tr}(\jmath(a)) = 2a_1, \quad \mathrm{tr}(\imath_1(a)) = \mathrm{tr}(\imath_2(a) = 4a_1, \tag{1.6}$$

$$\mathrm{eig}(a) := \mathrm{eig}(\jmath(a)) = [\sigma_+, \sigma_-], \tag{1.7}$$

$$\mathrm{eig}(\imath_1(a)) = \mathrm{eig}(\imath_2(a)) = [\sigma_+, \sigma_+, \sigma_-, \sigma_-], \text{ where}$$

$$\sigma_+ = a_1 + \sqrt{a_2^2 + a_3^2 + a_4^2}\,\mathbf{i} = a_1 + |a_v|\mathbf{i}, \quad \sigma_- = \overline{\sigma_+}, \tag{1.8}$$

$$|a| = ||\jmath(a)||_2 = ||\imath_1(a)||_2 = ||\imath_2(a)||_2, \tag{1.9}$$

$$\mathrm{cond}(a) := \mathrm{cond}(\jmath(a)) = \mathrm{cond}(\imath_1(a)) = \mathrm{cond}(\imath_2(a)) = 1, \tag{1.10}$$

$$\jmath(a\overline{a}) = \jmath(a)\jmath(a)^* = |a|^2\jmath(1) = |a|^2\mathbf{I}_2, \tag{1.11}$$

$$\imath_1(a\overline{a}) = \imath_1(a)\imath_1(a)^{\mathrm{T}} = \imath_2(a\overline{a}) = \imath_2(a)^{\mathrm{T}}\imath_2(a) = |a|^2\mathbf{I}_4, \tag{1.12}$$

where det, tr, eig, cond refer to *determinant, trace, collection of eigenvalues, condition*, respectively. By $\mathbf{I}_2, \mathbf{I}_4$ we denote the identity matrices of order 2 and 4, respectively.

We note that a general theory for determinants of quaternion valued matrices is not available. See [1, Fan, 2003]. We will review the classical matrix decompositions and investigate the applicability to quaternions. For the classical theory we usually refer to one of the books of Horn & Johnson, [3], [4].

In this connection it is useful to introduce another notion, namely that of equivalence between two quaternions. Such an equivalence may already be regarded as one of the important decompositions, namely the Schur decomposition, as we will see.

Definition 1.2. Two quaternions $a, b \in \mathbb{H}$ will be called *equivalent*, if there is an $h \in \mathbb{H}\backslash\{0\}$ such that

$$b = h^{-1}ah.$$

Equivalent quaternions a, b will be denoted by $a \sim b$. The set

$$[a] := \{s : s := h^{-1}ah,\ h \in \mathbb{H}\}$$

will be called *equivalence class of* a. It is the set of all quaternions which are equivalent to a.

Lemma 1.3. *The above defined notion of equivalence defines an equivalence relation. Two quaternions* a, b *are equivalent if and only if*

$$\Re a = \Re b, \quad |a| = |b|. \tag{1.13}$$

Furthermore, $a \in \mathbb{R} \Leftrightarrow \{a\} = [a]$. *Let* $a \in \mathbb{C}$. *Then* $\{a, \overline{a}\} \subset [a]$. *Let* $a = (a_1, a_2, a_3, a_4) \in \mathbb{H}$. *Then*

$$\sigma_+ := a_1 + \sqrt{a_2^2 + a_3^2 + a_4^2}\,\mathbf{i} \in [a].$$

Proof: [6]. □

The complex number σ_+ occurring in the last lemma will be called *complex representative of* $[a]$. The equivalence $a \sim b$ can be expressed also in the form $ah - hb = 0$, with an $h \neq 0$. This is the homogeneous form of Sylvester's equation. This equation was investigated by Janovská & Opfer[9]. It should be noted that algebraists refer to equivalent elements usually as *conjugate* elements. See [10, v. d. Waerden, 1960, p. 35].

2. Decompositions of quaternions. A matrix decomposition of the form $\jmath(a) = \jmath(b)\jmath(c)$ or $\jmath(a) = \jmath(b)\jmath(c)\jmath(d)$ with $a, b, c, d \in \mathbb{H}$ and the same with $\imath_1$ also represents a direct decomposition of the involved quaternions, namely $a = bc$ or $a = bcd$ because of the isomorphy of the involved mappings $\jmath, \imath_1$. The same applies to $\imath_2$, only the multiplication order has to be reversed. We will study the possibility of decomposing quaternions with respect to various well known matrix decompositions. A survey paper on decompositions of quaternionic matrices was given by [11, Zhang, 1997].

2.1. Schur decompositions. Let $\mathbf{U}$ be an arbitrary real or complex square matrix. If $\mathbf{U}\mathbf{U}^* = \mathbf{I}$ (identity matrix) then $\mathbf{U}$ will be called *unitary*. If $\mathbf{U}$ is real, then, $\mathbf{U}^* = \mathbf{U}^{\mathrm{T}}$. A real, unitary matrix will also be called *orthogonal*.

THEOREM 2.1. *(Schur 1) Let $\mathbf{A}$ be an arbitrary real or complex square matrix. Then there exists a unitary matrix $\mathbf{U}$ of the same size as $\mathbf{A}$ such that*

$$\mathbf{D} := \mathbf{U}^*\mathbf{A}\mathbf{U} \tag{2.1}$$

is an upper triangular matrix and as such contains the eigenvalues of $\mathbf{A}$ on its diagonal.

Proof: See HORN & JOHNSON[3, p. 79]. □

THEOREM 2.2. *(Schur 2) Let $\mathbf{A}$ be an arbitrary real square matrix of order n. Then there exists a real, orthogonal matrix $\mathbf{V}$ of order n such that*

$$\mathbf{H} := \mathbf{V}^{\mathrm{T}}\mathbf{A}\mathbf{V} \tag{2.2}$$

is an upper Hessenberg matrix with $k \le n$ block entries in the diagonal which are either real (1×1) matrices or real (2×2) matrices which have a pair of non real complex conjugate eigenvalues which are also eigenvalues of $\mathbf{A}$.

Proof: See HORN & JOHNSON[3, p. 82]. □

The representation $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^*$ implied by (2.1) is usually referred to as *complex Schur decomposition of* $\mathbf{A}$, whereas $\mathbf{A} = \mathbf{V}\mathbf{H}\mathbf{V}^{\mathrm{T}}$ implied by (2.2) is usually referred to as *real Schur decomposition of* $\mathbf{A}$. Let a be a quaternion, then we might ask whether there is a Schur decomposition of the matrices $\jmath(a), \imath_1(a), \imath_2(a)$ in terms of quaternions. The (affirmative) answer was already given by Janovská & Opfer[8, 2007].

THEOREM 2.3. *Let $a \in \mathbb{H}\backslash\mathbb{R}$ and σ_+ be the complex representative of $[a]$. There exists $h \in \mathbb{H}$ with $|h| = 1$ such that $\sigma_+ = h^{-1}ah$ and*

$$\jmath(a) = \jmath(h)\jmath(\sigma_+)\jmath(h^{-1}), \imath_1(a) = \imath_1(h)\imath_1(\sigma_+)\imath_1(h^{-1}), \imath_2(a) = \imath_2(h^{-1})\imath_2(\sigma_+)\imath_2(h) \tag{2.3}$$

are the Schur decompositions of $\jmath(a), \imath_1(a), \imath_2(a)$, respectively, which includes that $\jmath(h)$, $\imath_1(h), \imath_2(h)$ are unitary and $\jmath(h^{-1}) = \jmath(h)^*, \imath_1(h^{-1}) = \imath_1(h)^{\mathrm{T}}, \imath_2(h^{-1}) = \imath_2(h)^{\mathrm{T}}$. The first decomposition is complex, the other two are real.

Proof: The first two decompositions given in (2.3) follow immediately from Lemma 1.3 and the fact that $\jmath, \imath_1$ are isomorphisms. See [8]. The last equation can be written as $\imath_2(h)\imath_2(a) = \imath_2(\sigma_+)\imath_2(h)$. Applying (1.4) one obtains $ah = h\sigma_+$ which coincides with the equation for σ_+ given in the beginning of the theorem. Matrix $\jmath(\sigma_+)$ is complex and diagonal: $\jmath(\sigma_+) = \mathrm{diag}(\sigma_+, \sigma_-)$. The other matrices $\imath_1(\sigma_+), \imath_2(\sigma_+)$ are upper Hessenberg with two real (2×2) blocks each:

$$\imath_1(\sigma_+) = \begin{pmatrix} a_1 & -|a_v| & 0 & 0 \\ |a_v| & a_1 & 0 & 0 \\ 0 & 0 & a_1 & -|a_v| \\ 0 & 0 & |a_v| & a_1 \end{pmatrix}, \imath_2(\sigma_+) = \begin{pmatrix} a_1 & -|a_v| & 0 & 0 \\ |a_v| & a_1 & 0 & 0 \\ 0 & 0 & a_1 & |a_v| \\ 0 & 0 & -|a_v| & a_1 \end{pmatrix}. \square$$

If we have a look at the forms of $\imath_1$ and $\imath_2$, defined in (1.2), (1.3), respectively, we see that an upper (and lower) triangular matrix reduces immediately to a multiple of the identity matrix. This corresponds to the case where a is a real quaternion. Or in other words, it is not possible to find a complex Schur decomposition of $\imath_1(a), \imath_2(a)$ in $\mathbb{H}_\mathbb{R}, \mathbb{H}_\mathbb{P}$, respectively, if $a \notin \mathbb{R}$. In the mentioned paper [8, Section 8] we can also find, how to construct h which occurs in Theorem 2.3. One possibility is to put $h := \tilde{h}/|\tilde{h}|$, where

$$(2.4)\quad \tilde{h} := \begin{cases} (|a_v| + a_2, |a_v| + a_2, a_3 - a_4, a_3 + a_4) & \text{if } |a_3| + |a_4| > 0, \\ (1, 0, 0, 0) & \text{if } a_3 = a_4 = 0 \text{ and } a_2 > 0, \\ (0, 1, 0, 0) & \text{if } a_3 = a_4 = 0 \text{ and } a_2 < 0. \end{cases}$$

Let $\sigma_+ \sim a$ and multiply the defining equation $\sigma_+ = h^{-1}ah$ from the left by h, then $h\sigma_+ - ah = 0$ is the homogeneous form of Sylvester's equation and it was shown ([9]) that under the condition stated in (1.13) the homogeneous equation has a solution space (null space) which is a two dimensional subspace of $\mathbb{H}$ over $\mathbb{R}$.

2.2. The polar decomposition. The aim is to generalize the polar representation of a complex number. Let $z \in \mathbb{C}\backslash\{0\}$ be a complex number. Then, $z = |z|(z/|z|)$, and this representation of z is unique in the class of all two factor representations $z = pu$, where the first factor p is positive and the second, u, has modulus one. For matrices $\mathbf{A}$ one could correspondingly ask for a representation of the form $\mathbf{A} = \mathbf{PU}$, where the first factor $\mathbf{P}$ is positive semidefinite and the second, $\mathbf{U}$, is unitary. This is indeed possible, even for non square matrices $\mathbf{A} \in \mathbb{C}^{m\times n}, m \le n$. Matrix $\mathbf{P}$ is always uniquely defined as $\mathbf{P} = (\mathbf{AA}^*)^{1/2}$ and $\mathbf{U}$ is uniquely defined if $\mathbf{A}$ has maximal rank m. If $\mathbf{A}$ is square and non singular, then $\mathbf{U} = \mathbf{P}^{-1}\mathbf{A}$. See Horn & Johnson[3, Theorem 7.3.2 and Corollary 7.3.3, pp. 412/413].

Let $a \in \mathbb{H}\backslash\{0\}$ be a non vanishing quaternion $a := (a_1, a_2, a_3, a_4)$. The quantity $a_v := (0, a_2, a_3, a_4)$ was called vector part of a as previously explained. The matrices $\jmath(a), \imath_1(a), \imath_2(a)$ are non singular square matrices where the columns are orthogonal to each other. See (1.11), (1.12) and its representation (in terms of quaternions) is obviously

$$a = |a|\frac{a}{|a|}. \tag{2.5}$$

The corresponding matrix representation in $\mathbb{H}_\mathbb{C}, \mathbb{H}_\mathbb{R}, \mathbb{H}_\mathbb{P}$, can be easily deduced by using (1.1) to (1.3) and the properties listed in (1.11), (1.12). We obtain

$$\jmath(a) = \mathrm{diag}(|a|, |a|)\,\jmath(\frac{a}{|a|}), \tag{2.6}$$

$$\imath_1(a) = \mathrm{diag}(|a|, |a|, |a|, |a|)\,\imath_1(\frac{a}{|a|}), \tag{2.7}$$

$$\imath_2(a) = \mathrm{diag}(|a|, |a|, |a|, |a|)\,\imath_2(\frac{a}{|a|}). \tag{2.8}$$

In all cases the first factor is positive definite and the second is unitary, orthogonal, respectively.

From a purely algebraic standpoint this representation of a is complete. However, already the name *polar* representation means more. In the complex case we have

$$\frac{z}{|z|} = \exp(\alpha\mathbf{i}), \quad z \neq 0$$

where $\alpha := \arg z$ is the angle between the x-axis and an arrow representing z emanating from the origin of the z-plane. As formula: $\alpha = \arctan(\Im z/\Re z)$. In the quaternionic case one finds (cf. [2, Girard, 2007, p. 11]

$$\frac{a}{|a|} = \exp(\alpha u), \quad a \neq 0,$$

with $u := a_v/|a_v|, \alpha := \arctan(|a_v|/a_1)$, and exp is defined by its Taylor series using $u^2 = -1$.

2.3. The singular value decomposition (SVD). We start with the following well known theorem on a singular value decomposition of a given matrix $\mathbf{A}$. We restrict ourselves here to square matrices. The singular values of $\mathbf{A}$ are the square roots of the (non negative) eigenvalues of the positive semidefinite matrix $\mathbf{AA}^*$.

Theorem 2.4. *Let $\mathbf{A}$ be an arbitrary square matrix with real or complex entries. Then there are two unitary matrices $\mathbf{U}, \mathbf{V}$ of the same size as $\mathbf{A}$ such that*

$$\mathbf{D} := \mathbf{UAV}^*$$

is a diagonal matrix with the singular values of $\mathbf{A}$ in decreasing order on the diagonal. And the number of positive diagonal entries is the rank of $\mathbf{A}$.

Proof: See Horn & Johnson[3, 1991, p. 414]. □

Let a be a quaternion. The eigenvalues of $\jmath(a)$ are σ_+, σ_-, defined in (1.8) and

$$\jmath(a)\jmath(a)^* = \begin{pmatrix} |a|^2 & 0 \\ 0 & |a|^2 \end{pmatrix}.$$

Thus, the singular values of $\jmath(a)$ are $|a|, |a|$. The wanted decomposition must be of the form

$$\begin{pmatrix} |a| & 0 \\ 0 & |a| \end{pmatrix} = \mathbf{U} \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} \mathbf{V}^*$$

and the main question is whether $\mathbf{U}, \mathbf{V} \in \mathbb{H}_{\mathbb{C}}$. In order to solve this problem, we write it directly in terms of quaternions, namely

$$|a| = ua\overline{v}, \quad |u| = |v| = 1. \tag{2.9}$$

Theorem 2.5. *Let $a \in \mathbb{H}\backslash\mathbb{R}$. Choose $u \in \mathbb{H}$ with $|u| = 1$ and define $v := ua/|a|$ or, equivalently, choose v with $|v| = 1$ and define $u := v\overline{a}/|a|$. Then (2.9) defines a singular value decomposition of a and*

$$\jmath(|a|) = \jmath(u)\jmath(a)\jmath(v)^*$$

defines a corresponding SVD in $\mathbb{H}_{\mathbb{C}}$. A SVD with $u = v$ is impossible. The corresponding SVDs in $\mathbb{H}_{\mathbb{R}}$ and in $\mathbb{H}_{\mathbb{P}}$ are

$$\imath_1(|a|) = \imath_1(u)\imath_1(a)\imath_1(v)^{\mathrm{T}}, \quad \imath_2(|a|) = \imath_2(v)^{\mathrm{T}}\imath_2(a)\imath_2(u).$$

Proof: It is easy to see that (2.9) is valid if we choose u, v according to the given rules. If $u = v$ then $a = |a| \in \mathbb{R}$ follows, which was excluded. □

One very easy realization of (2.9) is to choose $u := 1$ and $v := a/|a|$ or to choose $v := 1$ and $u := \overline{a}/|a|$.

Example 2.6. *Let $a := (1, 2, 2, 4)$. Then the three SVDs are:*

$$\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1+2\mathbf{i} & 2+4\mathbf{i} \\ -2+4\mathbf{i} & 1-2\mathbf{i} \end{pmatrix} \begin{pmatrix} 1-2\mathbf{i} & -2-4\mathbf{i} \\ 2-4\mathbf{i} & 1+2\mathbf{i} \end{pmatrix} /5.$$

$$\begin{pmatrix} 5 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -2 & -2 & -4 \\ 2 & 1 & -4 & 2 \\ 2 & 4 & 1 & -2 \\ 4 & -2 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 2 & 4 \\ -2 & 1 & 4 & -2 \\ -2 & -4 & 1 & 2 \\ -4 & 2 & -2 & 1 \end{pmatrix} /5.$$

$$\begin{pmatrix} 5 & 0 & 0 & 0 \\ 0 & 5 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 2 & 4 \\ -2 & 1 & -4 & 2 \\ -2 & 4 & 1 & -2 \\ -4 & -2 & 2 & 1 \end{pmatrix} /5 \begin{pmatrix} 1 & -2 & -2 & -4 \\ 2 & 1 & 4 & -2 \\ 2 & -4 & 1 & 2 \\ 4 & 2 & -2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

2.4. The Jordan decomposition. Let $a := (a_1, a_2, a_3, a_4) \in \mathbb{H}\backslash\mathbb{R}$. Since the two eigenvalues $\sigma_\pm$ of $\jmath(a)$, defined in (1.8), are different there will be an $s \in \mathbb{H}\backslash\{0\}$ such that $a = s^{-1}\sigma_+ s$ which implies

$$\jmath(a) = \jmath(s^{-1})\jmath(\sigma_+)\jmath(s).$$

And this representation is the Jordan decomposition of $\jmath(a)$ and $\mathbf{J} := \jmath(\sigma_+) = \begin{pmatrix} \sigma_+ & 0 \\ 0 & \sigma_- \end{pmatrix}$ is the Jordan canonical form of $\jmath(a)$ ([3, Horn & Johnson, p. 126]). In this context this representation is almost the same as the Schur decomposition, only we do not require that $|s| = 1$. For the computation of s, we could use formula (2.4). In $\mathbb{H}_{\mathbb{C}}, \mathbb{H}_{\mathbb{P}}$ this decomposition reads

$$\imath_1(a) = \imath_1(s^{-1})\imath_1(\sigma_+)\imath_1(s), \quad \imath_2(a) = \imath_2(s)\imath_2(\sigma_+)\imath_2(s^{-1}),$$

where the explicit forms of $\imath_1(\sigma_+), \imath_2(\sigma_+)$ are given in the proof of Theorem 2.3.

2.5. The QR decomposition. Let $\mathbf{A}$ be an arbitrary complex square matrix. Then there is a unitary matrix $\mathbf{U}$ and an upper triangular matrix $\mathbf{R}$ of the same size as $\mathbf{A}$ such that

$$\mathbf{A} = \mathbf{U}\mathbf{R}.$$

This well known theorem can be found in ([3, Horn & Johnson, p. 112]). And this decomposition is referred to as *QR-decomposition of* $\mathbf{A}$. All triangular matrices in $\mathbb{H}_\mathbb{C}$, in $\mathbb{H}_\mathbb{R}$, and in $\mathbb{H}_\mathbb{P}$ reduce to diagonal matrices. Therefore, the QR-decompositions of a quaternion $a \neq 0$ have the trivial form

$$a = \frac{a}{|a|}\,|a| \Leftrightarrow \jmath(a) = \jmath\Big(\frac{a}{|a|}\Big)\,\jmath(|a|),\ \imath_1(a) = \imath_1\Big(\frac{a}{|a|}\Big)\,\imath_1(|a|),\ \imath_2(a) = \imath_2\Big(\frac{a}{|a|}\Big)\,\imath_2(|a|),$$

which is identical with the polar decomposition (2.5).

2.6. The LU decomposition. Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be given with entries $a_{jk},\ j,k = 1,2,\ldots,n$. Define the n submatrices $\mathbf{A}_\ell := (a_{jk}),\ j,k = 1,2,\ldots,\ell, \ell = 1,2,\ldots,n$. Then, following Horn & Johnson[3, p. 160] there is a lower triangular matrix $\mathbf{L}$ and an upper triangular matrix $\mathbf{U}$ such that

$$\mathbf{A} = \mathbf{L}\mathbf{U}$$

if and only if all n submatrices $\mathbf{A}_\ell,\ \ell = 1,2,\ldots,n$ are non singular. The above representation is called *LU-decomposition of* $\mathbf{A}$. Since triangular matrices in $\mathbb{H}_\mathbb{C}$, in $\mathbb{H}_\mathbb{R}$, and in $\mathbb{H}_\mathbb{P}$ reduce to diagonal matrices and since a product of two diagonal matrices is again diagonal an LU-decomposition of a quaternion a will in general not exist since $\jmath(a), \imath_1(a), \imath_2(a)$ are in general not diagonal. So we may ask for the ordinary LU-decomposion of $\jmath(a), \imath_1(a), \imath_2(a)$. In order that such a decomposition exist we must require that the mentioned submatrices are not singular. Let $a = (a_1, a_2, a_3, a_4)$. Then the two mentioned submatrices of $\jmath(a)$ are non singular if and only if the first (1×1) submatrix $\alpha := a_1 + a_2\mathbf{i} \neq 0$, since this implies that also the second (2×2) submatrix which is $\jmath(a)$ is non singular because its determinant is $|a|^2 = |\alpha|^2 + a_3^2 + a_4^2 > 0$.

Theorem 2.7. *Let $a = (a_1, a_2, a_3, a_4) \in \mathbb{H}$. Put $\alpha := a_1 + a_2\mathbf{i}$ and $\beta := a_3 + a_4\mathbf{i}$. An LU decomposition of $\jmath(a)$ exists if and only if $\alpha \neq 0$. If this condition is valid, then*

$$\jmath(a) = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ l_{21} & 1 \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ 0 & u_{22} \end{pmatrix},$$

where

$$l_{21} = -\frac{\overline{\beta}}{\alpha},$$
$$u_{22} = \frac{|\alpha|^2 + |\beta|^2}{\alpha} = \frac{|a|^2}{\alpha}.$$

Proof: The if and only part follows from the general theory. The above formula is easy to check. □

Theorem 2.8. *Let $a = (a_1, a_2, a_3, a_4) \in \mathbb{H}$. The four submatrices $\mathbf{A}_l$ of $\imath_1(a)$ and of $\imath_2(a)$ are non singular if and only if $a_1 \neq 0$. If this condition is valid, then*

$$\imath_1(a) := \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ a_2 & a_1 & -a_4 & a_3 \\ a_3 & a_4 & a_1 & -a_2 \\ a_4 & -a_3 & a_2 & a_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{pmatrix} \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix},$$

where [results for $\imath_2(a)$ are in parentheses]

$$\begin{aligned}
l_{j1} &:= a_j/a_1, j = 2,3,4, \quad (\textit{no change for } i_2(a)),\\
l_{32} &:= (a_1a_4 + a_2a_3)/(a_1^2 + a_2^2), \quad (l_{32} := (-a_1a_4 + a_2a_3)/(a_1^2 + a_2^2) \textit{ for } \imath_2(a)),\\
l_{42} &:= (a_2a_4 - a_1a_3)/(a_1^2 + a_2^2), \quad (l_{42} := (a_2a_4 + a_1a_3)/(a_1^2 + a_2^2) \textit{ for } \imath_2(a)),\\
u_{22} &:= (a_1^2 + a_2^2)/a_1, \quad (\textit{no change for } \imath_2(a)),\\
u_{23} &:= (-a_1a_4 + a_2a_3)/a_1, \quad (u_{23} := (a_1a_4 + a_2a_3)/a_1 \textit{ for } \imath_2(a)),\\
u_{24} &:= (a_1a_3 + a_2a_4)/a_1, \quad (u_{24} := (-a_1a_3 + a_2a_4)/a_1 \textit{ for } \imath_2(a)),\\
u_{33} &:= a_1 + l_{31}a_3 - l_{32}u_{23}, \quad (\textit{no change for } \imath_2(a)),\\
l_{43} &:= (a_2 + l_{41}a_3 - l_{42}u_{23})/u_{33}, \quad (l_{43} := (-a_2 + l_{41}a_3 - l_{42}u_{23})/u_{33} \textit{ for } \imath_2(a)),\\
u_{34} &:= -a_2 + l_{31}a_4 - l_{32}u_{24}, \quad (u_{34} := a_2 + l_{31}a_4 - l_{32}u_{24} \textit{ for } \imath_2(a)),\\
u_{44} &:= a_1 + l_{41}a_4 - l_{42}u_{24} - l_{43}u_{34}, \quad (\textit{no change for } \imath_2(a)).
\end{aligned}$$

A Cholesky decomposition cannot be achieved since all three matrices $\jmath(a), \imath_1(a), \imath_2(a)$ are missing symmetry.

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