Hamburger Beiträge
zur Angewandten Mathematik

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This paper has been submitted to
Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM)
The final form may differ from this preprint

Reihe A
Preprint 179
March 2004

Hamburger Beiträge zur Angewandten Mathematik

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The conjugate gradient algorithm applied to quaternion-valued matrices

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Abstract. The well known conjugate gradient algorithm (cg-algorithm), introduced by Hestenes & Stiefel, [1952] intended for real, symmetric, positive definite matrices works as well for complex matrices and has the same typical convergence behavior. It will also work, not generally, but in many cases for hermitean, but not necessarily positive definite matrices. We shall show, that the same behavior is still valid if we apply the cg-algorithm to matrices with quaternion entries. We particularly investigate the early stop of the cg-algorithm in this case and we develop error estimates. We have to present some basic facts about quaternions and about matrices with quaternion entries, in particular, about eigenvalues of such matrices. We also present some numerical examples of quaternion systems solved by the cg-algorithm.

Keywords. Quaternion-valued matrices, conjugate gradient algorithm, cg-algorithm, linear systems of equation with quaternion coefficients.

2000 MSC. 15A33, 65F10, 65F25.

1. Introduction

Let $\mathbf{A}$ be an ordinary square matrix and $\mathbf{b}, \mathbf{x}$ ordinary vectors where the lengths of $\mathbf{b}, \mathbf{x}$ are supposed to be the same as the order of the matrix $\mathbf{A}$, and where all entries of $\mathbf{A}$, $\mathbf{b}$, $\mathbf{x}$ may be complex. By $\mathbf{B}^*$, applied to an arbitrary complex matrix $\mathbf{B}$ we understand the transpose of the complex conjugate (applied elementwise) of the matrix $\mathbf{B}$. The transpose of a matrix $\mathbf{B}$ will be denoted by $\mathbf{B}^{\mathrm{T}}$. A matrix $\mathbf{B}$ will be called *hermitean* if $\mathbf{B} = \mathbf{B}^*$. Necessarily, a hermitean matrix is a square matrix. If a hermitean matrix $\mathbf{B}$ has the property that $\mathbf{x}^*\mathbf{A}\mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$, then, $\mathbf{B}$ will be called *positive definite*. If it has the property that $\mathbf{x}^*\mathbf{A}\mathbf{x} \geq 0$ for all $\mathbf{x} \in \mathbb{C}^n$, then, $\mathbf{B}$ will be called positive *semi definite*. The notations $\Re, \Im$ will be used for *real, imaginary part*, respectively, of what follows. If f is any real valued function (on an arbitrary non empty domain D) then, $f(x) = \min$ is an abbreviation for the problem of finding all (global) minima of f on D. One of the essential features of the classical conjugate gradient method is contained in the following theorem.

Theorem 1. For $\mathbf{A} \in \mathbb{C}^{n\times n}, \mathbf{b}, \mathbf{x} \in \mathbb{C}^n$ where $n \in \mathbb{N}$ let

$$f(\mathbf{x}) := \frac{1}{2}\mathbf{x}^*\mathbf{A}\mathbf{x} - \Re(\mathbf{b}^*\mathbf{x}), \tag{1}$$

$$g(\mathbf{x}) := \mathbf{A}\mathbf{x} - \mathbf{b}. \tag{2}$$

Assume that $\mathbf{A}$ is hermitean and positive definite. Then, each of the two problems

$$\text{(a)}: \quad f(\mathbf{x}) = \min, \qquad \text{(b)}: \quad g(\mathbf{x}) = \mathbf{0} \tag{3}$$

has a unique solution and these solutions coincide.

Proof: Problem (a) has a unique solution because of the strict convexity of f. Problem (b) has a unique solution since $\mathbf{A}$ is not singular. By simple computation for arbitrary $\mathbf{h}, \mathbf{x} \in \mathbb{C}^n$ we have

$$f(\mathbf{x}+\mathbf{h}) = f(\mathbf{x}) + f(\mathbf{h}) + \Re(\mathbf{h}^*\mathbf{A}\mathbf{x}). \tag{4}$$

(i) Let $g(\hat{\mathbf{x}}) = \mathbf{0}$. Then $f(\hat{\mathbf{x}}+\mathbf{h}) = f(\hat{\mathbf{x}}) + \frac{1}{2}\mathbf{h}^*\mathbf{A}\mathbf{h}$ or $f(\hat{\mathbf{x}}) = f(\hat{\mathbf{x}}+\mathbf{h}) - \frac{1}{2}\mathbf{h}^*\mathbf{A}\mathbf{h} < f(\hat{\mathbf{x}}+\mathbf{h})$ for all $\mathbf{h} \neq \mathbf{0}$. Thus, $\hat{\mathbf{x}}$ is the unique minimizer of f and $\hat{\mathbf{x}}$ solves problem (a). (ii) Let $\hat{\mathbf{x}}$ be a minimizer of f. Then, $f(\hat{\mathbf{x}}) \le f(\hat{\mathbf{x}}+\mathbf{h}) = f(\hat{\mathbf{x}})+f(\mathbf{h})+\Re(\mathbf{h}^*\mathbf{A}\hat{\mathbf{x}})$ for all $\mathbf{h}$ and therefore $f(\mathbf{h})+\Re(\mathbf{h}^*\mathbf{A}\hat{\mathbf{x}}) = \frac{1}{2}\mathbf{h}^*\mathbf{A}\mathbf{h} - \Re(\mathbf{b}^*\mathbf{h}) + \Re(\mathbf{h}^*\mathbf{A}\hat{\mathbf{x}}) = \Re(\mathbf{h}^*g(\hat{\mathbf{x}})) + \frac{1}{2}\mathbf{h}^*\mathbf{A}\mathbf{h} \ge 0$. Let $\mathbf{y} := g(\hat{\mathbf{x}}) \neq \mathbf{0}$ and put $\mathbf{h} := -\dfrac{\mathbf{y}^*\mathbf{y}}{\mathbf{y}^*\mathbf{A}\mathbf{y}}\,\mathbf{y}$. Then $\Re(\mathbf{h}^*g(\hat{\mathbf{x}}))+\frac{1}{2}\mathbf{h}^*\mathbf{A}\mathbf{h} = -\frac{1}{2}\dfrac{(\mathbf{y}^*\mathbf{y})^2}{\mathbf{y}^*\mathbf{A}\mathbf{y}} < 0$, a contradiction. Thus, $g(\hat{\mathbf{x}}) = \mathbf{0}$ and $\hat{\mathbf{x}}$ solves problem (b). □

The idea introduced by Hestenes & Stiefel, [1952] was, to solve (a) of (3) instead (b) by solving $\min_{\alpha\in\mathbb{R}} f(\mathbf{x}+\alpha\mathbf{d})$ repeatedly for varying and cleverly chosen *directions* $\mathbf{d}$. Since this story is well known, we present the final algorithm in the classical form. We start with a vector $\mathbf{x}_j$, its residual $\mathbf{r}_j$, a direction $\mathbf{d}_j$ and show how to compute the next vector $\mathbf{x}_{j+1}$, the next residual $\mathbf{r}_{j+1}$, and the next direction $\mathbf{d}_{j+1}$, $j = 0, 1, \ldots$

Program 2. cg-Algorithm: given $\mathbf{A}, \mathbf{b}, \mathbf{x}_0$

initial step=====================

$\mathbf{d}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0;$

$\mathbf{r}_0 = \mathbf{d}_0;$

$r_0 = \mathbf{r}_0^*\mathbf{r}_0;\ j = 0;$

loop starts: `while` $\mathbf{r}_j \neq \mathbf{0}$ `do`==========

$\mathbf{A}_\mathbf{d} = \mathbf{A}\mathbf{d}_j;$

$\alpha_j = r_j/(\mathbf{d}_j^*\mathbf{A}_\mathbf{d});$

$\mathbf{x}_{j+1} = \mathbf{x}_j + \alpha_j\mathbf{d}_j;$

$\mathbf{r}_{j+1} = \mathbf{r}_j - \alpha_j\mathbf{A}_\mathbf{d};$

$r_{j+1} = \mathbf{r}_{j+1}^*\mathbf{r}_{j+1};$

$\beta_j = r_{j+1}/r_j;$

$\mathbf{d}_{j+1} = \mathbf{r}_{j+1} + \beta_j\mathbf{d}_j;\ j = j + 1;$

loop ends=====================

The well known stopping behavior is given in the next theorem.

Theorem 3. Let $\mathbf{A} \in \mathbb{C}^{n\times n}$ be hermitean and positive definite. (a) The above algorithm stops (at the latest) after n steps with the joint solution of the problems mentioned in (3). (b) It already stops after (at most) $m \leq n$ steps with the solution if m is the number of different eigenvalues of $\mathbf{A}$.

Proof: Kelley, [1995, p. 14–15]. □

We want to show, that Theorem 1 and Theorem 3 remain true if the complex entries of the above $\mathbf{A}, \mathbf{b}$ are replaced with quaternions. We should also mention that part (b) of Theorem 3 does not originate from the Hestenes & Stiefel paper. It was first observed by Reid, [1971]. It seems appropriate and necessary to repeat some essential features of quaternions.

2. Excursion to quaternions

In the beginning of this section we repeat some elementary properties of quaternions. In the end we will mention some papers important in the development of quaternions. Let $\mathbb{H} := \mathbb{R}^4$ be equipped with the ordinary vector space structure and with an additional multiplicative structure

$\mathbb{H} \times \mathbb{H} \to \mathbb{H}$ which most easily can be defined by a multiplication table (see Table 4) for the four basis elements

$$(5) \quad \mathrm{h} := (1,0,0,0), \quad \mathrm{i} := (0,1,0,0), \quad \mathrm{j} := (0,0,1,0), \quad \mathrm{k} := (0,0,0,1).$$

Table 4. Multiplication table for quaternions

·	h	i	j	k
h	h	i	j	k
i	i	−h	k	−j
j	j	−k	−h	i
k	k	j	−i	−h

The letter $\mathbb{H}$ is chosen in honor of Hamilton[1)], who invented quaternions on Monday, October 16, 1843, cf. v. d. Waerden, [1973, p. 1]. It avoids the letter $\mathbb{Q}$ which is ordinarily used for the rationals. An element $h = (a,b,c,d) \in \mathbb{H}$ has then, the representation

$$(6) \qquad h := (a,b,c,d) = a\mathrm{h} + b\mathrm{i} + c\mathrm{j} + d\mathrm{k}.$$

Given h according to (6), the element denoted by $\overline{h}$ and defined by

$$(7) \qquad \overline{h} := (a,-b,-c,-d)$$

will be called the *conjugate* of h. The real number a will be called the *real part* of h and will be denoted by $\Re h$. The real number b will be called the i- or *imaginary part* and also denoted by $\Im h$, the number c will be called the j-part, the number d will be called the k-part of h. We define $\mathrm{vec}(h) := (0,b,c,d)$ and call it the *vector part* of h. A quaternion h with vanishing vector part will be identified with the real number $\Re h$ and if the j- and k-part are vanishing, h will be identified with the complex number $\Re h + \mathrm{i}\Im h$. By

$$(8) \qquad |h| := \sqrt{a^2+b^2+c^2+d^2}$$

we define the *absolute value* of h. With the multiplication as defined by Table 4 $\mathbb{H}$ becomes a non commutative field and it is known, that there is no multiplication in $\mathbb{R}^4$ which makes $\mathbb{R}^4$ a *commutative* field obeying *the law of moduli* (expression used by Hamilton, according to v. d. Waerden, [1973]) as expressed in the middle of (9), v. d. Waerden, [1955, p. 205]. It is easily checked that for two quaternions h_1, h_2 the product h_1h_2 is

[1)] Sir (1835) William Rowan Hamilton, 1805–1865, Irish mathematician, Professor of astronomy in Dublin.

commutative if one of the factors is real. This will be used frequently without further mentioning. To compute the product $h_1 h_2$ of two arbitrary quaternions h_1, h_2 16 multiplications and 12 additions of real numbers are necessary or in short: 28 *flops* are required. Thus, the computation of a scalar product of two quaternion-valued vectors with n components requires $32n$ (real) flops. We have

$$(9) \qquad |h|^2 = h\overline{h} = \overline{h}h, \quad |h_1 h_2| = |h_2 h_1| = |h_1||h_2|, \quad \overline{h_1 h_2} = \overline{h_2}\,\overline{h_1}$$

where we have applied the identification of $\overline{h}h$ with the real and non negative number $|h|^2$. The middle part of (9) makes $\mathbb{H}$ a *normed* vector space over $\mathbb{H}$ where the norm is introduced in (8). The space $\mathbb{H}^n$ becomes also a normed vector space. To see this, let $\mathbf{x} \in \mathbb{H}^n$ with $\mathbf{x} := (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ and define

$$(10) \qquad ||\mathbf{x}|| := \sqrt{\sum_{j=1}^{n} |x_j|^2}.$$

By means of (9) it is easily verified, that $\mathbb{H}^n$ becomes a normed space over $\mathbb{H}$. Now, let $\mathbf{B} \in \mathbb{H}^{m \times n}$ be a matrix with quaternion entries. Then, it is a representation of a linear mapping only in a restricted sense. The additivity $\mathbf{B}(\mathbf{x} + \mathbf{y}) = \mathbf{B}\mathbf{x} + \mathbf{B}\mathbf{y}$ is still true. But in general $\mathbf{B}(h\mathbf{x}) = h\mathbf{B}\mathbf{x}$ is not true since $\big(\mathbf{B}(h\mathbf{x})\big)_j = \sum_k b_{jk} h x_k \neq h \sum_k b_{jk} x_k$. But it is clear that $\mathbf{B}(\mathbf{x}h) = (\mathbf{B}\mathbf{x})h$. Thus, $\mathbf{B}$ represents a linear mapping with respect to multiplication from the right. With the definition (7) it is clear how to define $\mathbf{B}^*$, namely by forming the conjugates elementwise and then, transposing the resulting matrix. In case $\mathbf{B} = \mathbf{B}^*$, which can happen only for square matrices, $\mathbf{B}$ is called *hermitean*. A hermitean matrix is called *positive definite* if $\mathbf{x}^*\mathbf{B}\mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{H}^n \backslash \{\mathbf{0}\}$.
Since eigenvalues are involved in Theorem 3 we also introduce eigenvalues of square matrices $\mathbf{B}$ with quaternion entries.

Definition 5. Let $\mathbf{B} \in \mathbb{H}^{n \times n}$. If there is a vector $\mathbf{x} \in \mathbb{H}^n \backslash \{\mathbf{0}\}$ and a quaternion $\lambda \in \mathbb{H}$ such that

$$(11) \qquad \mathbf{B}\mathbf{x} = \mathbf{x}\lambda,$$

we call λ an *eigenvalue* of $\mathbf{B}$, and $\mathbf{x}$ an *eigenvector corresponding* to λ.

Let us point out that in the above definition we have put λ as a right factor of $\mathbf{x}$. This is in coincidence with the fact that $\mathbf{B}$ represents a linear mapping with respect to multiplication from the right. In the literature, e. g. ZHANG, [1997] one finds the definition of left and right eigenvalues, where the left eigenvalues play a sort of exotic role. If we multiply the defining equation (11) from the right by any $h \in \mathbb{H}\backslash\{0\}$ and replace $\mathbf{x}$ by $\mathbf{x}hh^{-1}$ we obtain $\mathbf{B}(\mathbf{x}h)h^{-1}h = (\mathbf{x}h)(h^{-1}\lambda h)$. Thus, $h^{-1}\lambda h$ is an eigenvalue corresponding to $\mathbf{x}h$. Therefore, with λ the whole *equivalence class*

$$[\lambda] := \left\{s : \ s := h^{-1}\lambda h, \quad h \in \mathbb{H}\backslash\{0\}\right\} \tag{12}$$

consists of eigenvalues. The number of eigenvalues is therefore not finite in general. However, the number of equivalence classes is at most n. This will be shown immediately. Two eigenvalues λ_1, λ_2 will be called *equivalent*, in signs $\lambda_1 \sim \lambda_2$, if they are residing in the same equivalence class. Two eigenvalues λ_1, λ_2 are equivalent if and only if $\Re\lambda_1 = \Re\lambda_2$ and $|\lambda_1| = |\lambda_2|$. Thus, if $\lambda = (a, b, c, d)$ is an eigenvalue, there is an equivalent eigenvalue $\tilde{\lambda} \sim \lambda$ with $\tilde{\lambda} = (a, +\sqrt{b^2 + c^2 + d^2}, 0, 0)$. Hence, if λ is not real then, in $[\lambda]$ there is exactly one complex eigenvalue with positive imaginary part. In particular, λ and $\overline{\lambda}$ are equivalent. That the number of equivalence classes is at most n will be shown in the next lemma.

Lemma 6. Let $\mathbf{B} \in \mathbb{H}^{n\times n}$. Then, the number of equivalence classes of eigenvalues of $\mathbf{B}$ is at most n.

Proof: Let λ_1, λ_2 be two non equivalent eigenvalues and $\mathbf{u}_1, \mathbf{u}_2$ corresponding eigenvectors. We shall show that $\mathbf{u}_1, \mathbf{u}_2$ are (right) linearly independent. Assume the contrary. I. e. there are quaternion constants $\alpha_1 \neq 0, \alpha_2 \neq 0$ with $\mathbf{u}_1\alpha_1 + \mathbf{u}_2\alpha_2 = \mathbf{0}$ or equivalently $\mathbf{u}_1 = \mathbf{u}_2\alpha$ where $\alpha := -\alpha_2(\alpha_1)^{-1} \neq 0$. Then, by multiplying with $\mathbf{B}$ from the left, we obtain $\mathbf{B}\mathbf{u}_1 = \mathbf{B}\mathbf{u}_2\alpha$ or $\mathbf{u}_1\lambda_1 = \mathbf{u}_2\lambda_2\alpha = \mathbf{u}_2\alpha\lambda_1$ or $\alpha\lambda_1 = \lambda_2\alpha$. Thus, λ_1, λ_2 are equivalent, a contradiction. Therefore, the number of equivalence classes is restricted by the maximal number of right independent vectors of $\mathbb{H}^n$, which is n. $\square$

We should remark that the classical proof employing the characteristic polynomial is not working, since the underlying theory of determinants does not carry over to quaternion-valued matrices. In addition, polynomials in $\mathbb{H}[x]$ do not have finitely many zeros, as well.

Thus, we can summarize: An arbitrary square matrix $\mathbf{B} \in \mathbb{H}^{n\times n}$ possesses at most n different eigenvalues with the following properties: The eigenvalues are either real or complex. If they are complex, then, the imaginary part is positive. There is the following consequence: If a matrix (with quaternion entries) has only real eigenvalues, then, the number of different eigenvalues is at most n. Therefore, the following theorem is very useful.

Theorem 7. Let $\mathbf{A} \in \mathbb{H}^{n\times n}$ be hermitean. Then, $\mathbf{A}$ has only real eigenvalues and the number of different eigenvalues is at most n. If in addition, $\mathbf{A}$ is positive definite, then, all eigenvalues are positive.

Proof: For $\mathbf{x} \neq \mathbf{0}$ let $\mathbf{Ax} = \mathbf{x}\lambda$. Multiplying from the left by $\mathbf{x}^*$ yields $\mathbf{x}^*\mathbf{Ax} = ||\mathbf{x}||^2\lambda$. Going to the quaternion conjugate gives $||\mathbf{x}||^2\lambda = ||\mathbf{x}||^2\overline{\lambda}$ since $\mathbf{A} = \mathbf{A}^*$. Therefore, λ is real and in case $\mathbf{A}$ is positive definite, λ is positive. □

Matrices with quaternion entries were investigated by Wolf, [1936], Lee, [1949], Brenner, [1951], Wiegmann, [1955]. In particular, various canonical forms known for real or complex matrices were also discovered for matrices with quaternion entries. In a newer paper, Zhang, [1997] gave a summary on those and newer results. In a recent paper Zhang & Wei, [2001] discussed the Jordan canonical form for quaternion matrices again and pointed out an error in Wiegmann's proof. The only paper related to numerical linear algebra is (apparently) due to Bunse-Gerstner, Byers, & Mehrmann, [1989]. They treat the qr-algorithm, present programs, but no examples. It is easy to see that also in the case of quaternion entries similar matrices have the same set of eigenvalues and upper triangular matrices have eigenvalues which can be read from the diagonal. This will be used in the sequel. In particular, the existence of the Schur canonical form allows us to write the eigenvalues of an arbitrary matrix in $\mathbb{H}^{n\times n}$ in the form $\lambda_1, \lambda_2, \ldots, \lambda_n$ where $\lambda_j \in \mathbb{R}$ or $\lambda_j \in \mathbb{C}$ with $\Im\lambda_j > 0, j = 1, 2, \ldots, n$. Quaternions with zero real part play an important role in the description of the movement of rigid bodies in $\mathbb{R}^3$, see Kuipers, [1999]. Applications also to other fields of physics can be found in Freguglia & Turchetti [2002] and in Dongarra, Gabriel, Koelling, & Wilkinson, [1984].

3. The conjugate gradient algorithm for quaternion-valued matrices

First we observe without difficulties that Theorem 1 remains true, if $\mathbf{A}, \mathbf{b}$ have quaternion entries and if $\mathbf{A}$ is hermitean and positive definite. The definition of f in (1) yields again a strictly convex function since in the proof only multiplications with real numbers are involved. It is known, that also in the quaternion case a hermitean, positive definite matrix is non singular (Zhang, [1997]), so the function g defined in (2) has a unique zero. The remaining part of the given proof can be repeated directly for the quaternion case, since all occurring scalar multiplications again involve only real numbers. We introduce a scalar product in $\mathbb{H}^n$ which is of the form

(13)

$$<\mathbf{x},\mathbf{y}>:=\sum_{j=1}^{n}\overline{y_j}x_j,\ \mathbf{x}:=(x_1,x_2,\ldots,x_n)^{\mathrm{T}},\ \mathbf{y}:=(y_1,y_2,\ldots,y_n)^{\mathrm{T}}\in\mathbb{H}^n.$$

It has the following properties:

(14a) $\quad <\mathbf{x}_1+\mathbf{x}_2,\mathbf{y}>=<\mathbf{x}_1,\mathbf{y}>+<\mathbf{x}_2,\mathbf{y}>,\quad \mathbf{x}_1,\mathbf{x}_2,\mathbf{y}\in\mathbb{H}^n,$

(14b) $\quad <\mathbf{x}\lambda,\mathbf{y}>=<\mathbf{x},\mathbf{y}>\lambda,\quad \lambda\in\mathbb{H},\ \mathbf{x},\mathbf{y}\in\mathbb{H}^n,$

(14c) $\quad <\mathbf{y},\mathbf{x}>=\overline{<\mathbf{x},\mathbf{y}>},\quad \mathbf{x},\mathbf{y}\in\mathbb{H}^n,$

(14d) $\quad <\mathbf{x},\mathbf{x}>=:||\mathbf{x}||^2>0$ for all $\mathbf{x}\in\mathbb{H}^n\backslash\{\mathbf{0}\}$.

These rules imply $<\mathbf{x},\mathbf{y}\lambda>=\overline{\lambda}<\mathbf{x},\mathbf{y}>$. They also imply additivity in the second component, i. e. $<\mathbf{x},\mathbf{y}_1+\mathbf{y}_2>=<\mathbf{x},\mathbf{y}_1>+<\mathbf{x},\mathbf{y}_2>$. In matrix terms the above scalar product can be written as

$$<\mathbf{x},\mathbf{y}>=\mathbf{y}^*\mathbf{x}\quad\Rightarrow\quad||\mathbf{x}||^2=<\mathbf{x},\mathbf{x}>=\mathbf{x}^*\mathbf{x}.$$

Let $\mathbf{B}$ be a hermitean, positive definite matrix. Then, we can also introduce

(15) $$<\mathbf{x},\mathbf{y}>_{\mathbf{B}}:=\mathbf{y}^*\mathbf{B}\mathbf{x}\quad\Rightarrow\quad||\mathbf{x}||_{\mathbf{B}}^2:=<\mathbf{x},\mathbf{x}>_{\mathbf{B}}=\mathbf{x}^*\mathbf{B}\mathbf{x}.$$

This product $<\mathbf{x},\mathbf{y}>_{\mathbf{B}}$ obeys the same rules (14a)–(14d) as the above introduced scalar product $<\mathbf{x},\mathbf{y}>$. Conversely, any form $\mathbb{H}^n\times\mathbb{H}^n\to\mathbb{H}$ which obeys the rules (14a)–(14d) is a scalar product of type (15). See, Horn & Johnson, [1992, p. 410] for the analog complex case. It should be noticed, that in (15) in general $||\mathbf{x}||_{\mathbf{B}}\neq||\overline{\mathbf{x}}||_{\mathbf{B}}$. However, that is not due to the quaternion character of the vector- and matrix entries. This will already happen for complex entries.

Example 8. Define

$$\mathbf{B}:=\begin{pmatrix}39 & 12+16\mathrm{i}\\ 12-16\mathrm{i} & 95\end{pmatrix},\quad \mathbf{z}:=\begin{pmatrix}3-\mathrm{i}\\ 5+7\mathrm{i}\end{pmatrix}.$$

Then, $||\mathbf{z}||_{\mathbf{B}}^2 = \mathbf{z}^*\mathbf{B}\mathbf{z} = 6780$ and $||\overline{\mathbf{z}}||_{\mathbf{B}}^2 = \mathbf{z}^{\mathrm{T}}\mathbf{B}\overline{\mathbf{z}} = 8444$.

Now it is clear, that two non zero quaternion-valued vectors $\mathbf{x}, \mathbf{y}$ are called *conjugate* (with respect to $\mathbf{B}$) if $< \mathbf{x}, \mathbf{y} >_{\mathbf{B}} = 0$. Because of (14c) two conjugate vectors $\mathbf{x}, \mathbf{y}$ also obey $< \mathbf{y}, \mathbf{x} >_{\mathbf{B}} = 0$. So the definition is symmetric. Since the derivation of the conjugate gradient method is based on the consecutive minimization of the real function $\varphi : \mathbb{R} \to \mathbb{R}$ defined by $\varphi(\alpha) := f(\mathbf{x} + \alpha\mathbf{d})$ the non commutativity of $\mathbb{H}$ is at no place crucial.

Theorem 9. Let $\mathbf{A} \in \mathbb{H}^{n\times n}, \mathbf{b} \in \mathbb{H}^n$ be given and let $\mathbf{A}$ be hermitean and positive definite. Then, the given cg-algorithm (Program 2) is still applicable and it will stop with the solution after (at most) n steps independent of the initial choice $\mathbf{x}_0$.

Proof: After n steps the constructed directions $\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_n$ span $\mathbb{H}^n$ since they are mutually conjugate (to be shown with standard techniques) and we shall therefore arrive at the solution after n steps. The essential point is that the non commutativity of $\mathbb{H}$ is at no point crucial, since all scalar multiplications in the algorithm are by real numbers which commute with quaternions. □

It is nevertheless not straightforward to apply Program 2 to quaternion-valued matrices, since almost all given operations are not generally found in programming languages. The following detailed example shows in addition to the final result the intermediate results and can be used for comparisons. Examples with higher numbers of variables will be presented in the end of this paper in order to show the speed of the descent of the residual vectors measured in the Euclidean norm.

Example 10. Let $\mathbf{A} = (a_{jk}),\ j,k = 1,2,3,4$ as follows:

$$\mathbf{A} := \left(\begin{array}{rrrrrrrrrr} a_{11} & a_{12} & a_{13} & a_{14} & a_{22} & a_{23} & a_{24} & a_{33} & a_{34} & a_{44} \\ \hline 128 & -20 & -44 & -17 & 140 & -8 & 7 & 128 & 81 & 112 \\ 0 & -15 & -48 & -58 & 0 & -8 & -12 & 0 & 31 & 0 \\ 0 & 10 & 26 & -3 & 0 & -22 & -25 & 0 & 19 & 0 \\ 0 & -4 & -8 & -20 & 0 & 1 & 22 & 0 & 27 & 0 \end{array}\right).$$

For the six missing elements a_{kj} we have $a_{kj} = \overline{a_{jk}},\ 1 \leq j < k \leq 4$. The matrix is positive definite and it has four different positive eigenvalues: 11.1266, 68.5920, 147.0928, 281.1886. The right hand side $\mathbf{b} =$

$(b_1, b_2, b_3, b_4)^{\mathrm{T}}$ is chosen in such a way that all four components of the solution are identical to $(2, 3, 4, 5)$. Explicitly, $b_1 = (485, 192, 763, -412), b_2 = (346, -46, 468, 800), b_3 = (-177, 584, 325, 1156), b_4 = (358, 788, 468, 986)$. The start vector is $\mathbf{x}_0 := (\mathrm{h}, \mathrm{h}, \mathrm{h}, \mathrm{h})^{\mathrm{T}}$, where h is defined in (5).

Step 1: $\alpha = 3.9324 \cdot 10^{-3}, \beta = 6.5864 \cdot 10^{-2}, ||\mathbf{r}|| = 5.9856 \cdot 10^2$,

$$\mathbf{x} = \left(\begin{array}{rrrr} x_1 & x_2 & x_3 & x_4 \\ \hline 2.7224 & 1.8927 & -0.31343 & 1.6882 \\ 1.2308 & -0.16123 & 1.9544 & 2.9454 \\ 2.8707 & 2.0645 & 1.2190 & 1.8050 \\ -1.4943 & 3.0398 & 4.4122 & 3.9914 \end{array}\right),$$

$$\mathbf{d} = \left(\begin{array}{rrrr} d_1 & d_2 & d_3 & d_4 \\ \hline -124.44 & 89.181 & 86.252 & 68.912 \\ 111.92 & 204.74 & -129.22 & 172.27 \\ 148.55 & 153.32 & 169.86 & 7.8767 \\ 350.39 & 214.51 & 45.091 & -10.478 \end{array}\right).$$

Step 2: $\alpha = 1.0326 \cdot 10^{-2}, \beta = 1.5312 \cdot 10^{-1}, ||\mathbf{r}|| = 2.3422 \cdot 10^2$,

$$\mathbf{x} = \left(\begin{array}{rrrr} x_1 & x_2 & x_3 & x_4 \\ \hline 1.4374 & 2.8136 & 0.57726 & 2.3998 \\ 2.3866 & 1.9530 & 0.62006 & 4.7243 \\ 4.4047 & 3.6478 & 2.9731 & 1.8863 \\ 2.1240 & 5.2549 & 4.8778 & 3.8832 \end{array}\right),$$

$$\mathbf{d} = \left(\begin{array}{rrrr} d_1 & d_2 & d_3 & d_4 \\ \hline 41.777 & -101.34 & 48.474 & 43.484 \\ 15.588 & 31.125 & 5.2703 & 45.196 \\ -9.0829 & -1.3378 & 90.199 & 49.794 \\ 147.70 & -82.911 & 57.618 & 39.562 \end{array}\right).$$

Step 3: $\alpha = 9.2111 \cdot 10^{-3}, \beta = 4.5285 \cdot 10^{-2}, ||\mathbf{r}|| = 4.9842 \cdot 10$,

$$\mathbf{x} = \left(\begin{array}{rrrr} x_1 & x_2 & x_3 & x_4 \\ \hline 1.8222 & 1.8801 & 1.0238 & 2.8003 \\ 2.5301 & 2.2397 & 0.66861 & 5.1406 \\ 4.3210 & 3.6355 & 3.8039 & 2.3450 \\ 3.4844 & 4.4912 & 5.4085 & 4.2476 \end{array}\right),$$

$$\mathbf{d} = \begin{pmatrix} d_1 & d_2 & d_3 & d_4 \\ \hline 2.0996 & 1.4156 & 11.527 & -9.4496 \\ 5.5477 & 8.9768 & 27.527 & -25.275 \\ -3.7904 & 4.3037 & 2.3148 & 19.541 \\ 17.894 & 6.0072 & -4.8235 & 8.8837 \end{pmatrix}.$$

Step 4: $\alpha = 8.4694 \cdot 10^{-2}, \beta = 1.0557 \cdot 10^{-26}, ||\mathbf{r}|| = 5.1211 \cdot 10^{-12}$,

$$\mathbf{x} = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 \\ \hline 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 \\ 4 & 4 & 4 & 4 \\ 5 & 5 & 5 & 5 \end{pmatrix},$$

$$\mathbf{d} = \begin{pmatrix} d_1 & d_2 & d_3 & d_4 \\ \hline -1.7666 \cdot 10^{-12} & 7.3541 \cdot 10^{-13} & -3.0198 \cdot 10^{-14} & -2.7534 \cdot 10^{-13} \\ 1.1680 \cdot 10^{-12} & -3.3751 \cdot 10^{-13} & -1.9824 \cdot 10^{-12} & -1.5312 \cdot 10^{-12} \\ -8.6109 \cdot 10^{-13} & 1.2967 \cdot 10^{-13} & 2.1736 \cdot 10^{-12} & 2.2702 \cdot 10^{-12} \\ -1.3003 \cdot 10^{-12} & -1.2292 \cdot 10^{-12} & 5.2669 \cdot 10^{-13} & -7.8693 \cdot 10^{-13} \end{pmatrix}.$$

4. The early stopping of the cg-algorithm

The only remaining part is (b) of Theorem 3, asserting an earlier stop in case the number m of different eigenvalues is less than n. In the classical case the cg-algorithm is identified as a polynomial based iteration (Fischer, [1996, p. 161]) and the conclusion is drawn from a minimal property of the polynomials considered. As we have already seen, matrices may have infinitely many eigenvalues. However, hermitean matrices which are the only type of matrix we are considering have n real eigenvalues. Let us shortly consider polynomials. Take as an example

(16) $$p(x) := x^2 + \mathrm{h},\ x \in \mathbb{H} \text{ and h is defined in (5).}$$

As we easily see from the multiplication table, Table 4 there are at least the six zeros $\pm\mathrm{i}, \pm\mathrm{j}, \pm\mathrm{k}$. But the general situation is worse. Let

(17) $$p(x) := \sum_{j=0}^{n} a_j x^j, \quad a_j \in \mathbb{R},\ x \in \mathbb{H}$$

be a polynomial with real coefficients defined for quaternions x. Then, for an arbitrary $h \in \mathbb{H}\backslash\{0\}$ we have

$$p(h^{-1}xh) = \sum_{j=0}^{n} a_j (h^{-1}xh)^j = \sum_{j=0}^{n} a_j \underbrace{(h^{-1}xh)(h^{-1}xh)\cdots(h^{-1}xh)}_{j \text{ times}}$$
$$= \sum_{j=0}^{n} a_j h^{-1} x^j h = h^{-1} p(x) h$$

since a_j and h^{-1} commute because all a_j are real. Thus, if x is a zero of p defined in (17), then, the whole equivalence class $[x]$ (defined in (12)) consists of zeros. The only case where $[x]$ consists only of the element x alone is where x is real.

In order to determine the early stopping rule, we have to introduce some more notation. Let us assume that the given cg-algorithm, Program 2 produces vectors $\mathbf{x}_j, \mathbf{r}_j, \mathbf{d}_j$, and real numbers $\alpha_j, \beta_j, j = 0, 1, \ldots$

We define the spaces (where all spans $\langle\cdots\rangle$ are real spans)

$$\mathcal{D}_{j+1} := \langle \mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_j \rangle,$$
$$\mathcal{R}_{j+1} := \langle \mathbf{r}_0, \mathbf{r}_1, \ldots, \mathbf{r}_j \rangle,$$

and for an arbitrary matrix $\mathbf{B} \in \mathbb{H}^{n\times n}$, and an arbitrary vector $\mathbf{h} \in \mathbb{H}^n$ the so called *Krylov space*

$$\mathcal{K}(\mathbf{B}, \mathbf{h}, j+1) := \langle \mathbf{h}, \mathbf{B}\mathbf{h}, \ldots, \mathbf{B}^j \mathbf{h} \rangle.$$

Because of lines `10` and `2` of Program 2 we have

$$\mathcal{D}_{j+1} = \mathcal{R}_{j+1}, j = 0, 1, \ldots, n-1. \tag{18}$$

By an inductive argument, using line `7` of Program 2 and (18) one can show, that

$$\mathcal{R}_{j+1} = \mathcal{K}(\mathbf{A}, \mathbf{d}_0, j+1). \tag{19}$$

This is particularly important. It says, that the stopping of the cg-algorithm with $\mathbf{r}_m = \mathbf{0}$ will happen if $\dim \mathcal{K}(\mathbf{A}, \mathbf{d}_0, j+1) = m$ for all $j \geq m$. Let $\hat{\mathbf{x}}$ be the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$. We define $\mathbf{e}_j = \hat{\mathbf{x}} - \mathbf{x}_j$, the *error* of the

j-th approximation. Then, from line 6 of Program 2 we obtain $\hat{\mathbf{x}} - \mathbf{x}_{j+1} = \hat{\mathbf{x}} - \mathbf{x}_j - \alpha_j \mathbf{d}_j$ or

$$\mathbf{e}_{j+1} = \mathbf{e}_j - \alpha_j \mathbf{d}_j = \mathbf{e}_0 - \sum_{k=0}^{j} \alpha_k \mathbf{d}_k$$

or using (18) and (19)

$$\mathbf{e}_{j+1} - \mathbf{e}_0 \in \mathcal{D}_{j+1} = \mathcal{K}(\mathbf{A}, \mathbf{d}_0, j+1).$$

Since $\mathbf{d}_0 = \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0 = \mathbf{A}\mathbf{e}_0$ we have

$$\mathbf{e}_{j+1} - \mathbf{e}_0 \in \langle \mathbf{A}\mathbf{e}_0, \mathbf{A}^2\mathbf{e}_0, \ldots, \mathbf{A}^{j+1}\mathbf{e}_0 \rangle. \tag{20}$$

We introduce the following notation:

$$\overline{\Pi}_j := \{p \in \Pi_j : p(0) = 1,\ p \text{ has real coefficients}\}, \quad j = 0, 1, \ldots \tag{21}$$

In other words, $\overline{\Pi}_j$ is the set of all polynomials of degree at most j with real coefficients and with constant term one. With this notation relation (20) means, that there is a certain matrix polynomial p such that

$$\mathbf{e}_j = p(\mathbf{A})\mathbf{e}_0, \quad p \in \overline{\Pi}_j,\ j = 0, 1, \ldots \tag{22}$$

If we multiply this equation from the left by $\mathbf{A}$ and use that the coefficients of p are real we obtain the almost identical equation

$$\mathbf{r}_j = p(\mathbf{A})\mathbf{r}_0, \quad p \in \overline{\Pi}_j,\ j = 0, 1, \ldots \tag{23}$$

For our theoretical purposes, we can slightly reformulate the function f to be minimized (introduced in (1)) by introducing the (unknown) error $\mathbf{e} := \hat{\mathbf{x}} - \mathbf{x}$, where $\hat{\mathbf{x}}$ is the solution of $\mathbf{A}\mathbf{x} = \mathbf{b}$. We have

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{e}^*\mathbf{A}\mathbf{e} + \frac{1}{2}\hat{\mathbf{x}}^*\mathbf{b}.$$

Since $\frac{1}{2}\hat{\mathbf{x}}^*\mathbf{b}$ is constant, we can as well minimize the function

$$\tilde{f}(\mathbf{x}) := \mathbf{e}^*\mathbf{A}\mathbf{e} = ||\mathbf{e}||_{\mathbf{A}}^2, \quad \mathbf{e} := \hat{\mathbf{x}} - \mathbf{x} \tag{24}$$

rather than the function f. Since $\mathbf{A}$ is positive definite, $\tilde{f}$ is uniquely minimized by $\mathbf{e} = \mathbf{0}$ and the minimal value is $\tilde{f}(\hat{\mathbf{x}}) = 0$. The minimization of $\tilde{f}$ in step j is in view of (22), (24) equivalent to the problem

$$\min_{p \in \overline{\Pi}_j} ||p(\mathbf{A})\mathbf{e}_0||_{\mathbf{A}}, \quad j = 1, 2, \ldots \tag{25}$$

With this interpretation, it is now easy to show that the cg-algorithm will stop after at most m steps, if the spectrum of $\mathbf{A}$ consists of m different eigenvalues, where $1 \leq m \leq n$. We have to repeat some information on normal matrices. A matrix $\mathbf{B} \in \mathbb{H}^{n \times n}$ is defined to be *normal* if $\mathbf{B}^*\mathbf{B} = \mathbf{B}\mathbf{B}^*$. Like in the real or complex case $\mathbf{B}$ is normal (ZHANG, [1997, p. 41]) if and only if it is orthogonally diagonalizable. In this case there is an orthogonal matrix $\mathbf{U} \in \mathbb{H}^{n \times n}$ in the sense $\mathbf{U}^*\mathbf{U} = \mathbf{U}\mathbf{U}^* = \mathbf{I}$, such that $\Delta := \mathbf{U}^*\mathbf{B}\mathbf{U}$ is a diagonal matrix where the diagonal entries are the complex eigenvalues of $\mathbf{B}$, all having non negative imaginary parts and the columns of $\mathbf{U}$ are corresponding eigenvectors. In case $\mathbf{B}$ is hermitean, the diagonal elements of Δ are all real.

Theorem 11. Let $\mathbf{A} \in \mathbb{H}^{n \times n}$ be a hermitean and positive definite matrix, $\sigma(\mathbf{A})$ its spectrum and $m := \#\sigma(\mathbf{A})$. Then, the given cg-algorithm (Program 2) will stop with the solution after (at most) m steps independent of the initial choice $\mathbf{x}_0$.

Proof: The matrix $\mathbf{A}$ is normal, thus, possesses an orthogonal matrix $\mathbf{U}$ of eigenvectors. Denote the columns by $\mathbf{u}_k, k = 1, 2, \ldots, n$. Then, there is a unique expansion of $\mathbf{e}_0$ in the form $\mathbf{e}_0 = \sum_{k=1}^{n} \mathbf{u}_k \beta_k$ with uniquely defined quaternions β_k. Then, $p(\mathbf{A})\mathbf{e}_0 = \sum_{k=1}^{n} p(\lambda_k)\mathbf{u}_k\beta_k$ where λ_k is an eigenvalue corresponding to $\mathbf{u}_k$. Let $\sigma(\mathbf{A}) = \{0 < \lambda_1 < \lambda_2 < \cdots < \lambda_m\}$. Then, the polynomial p defined by $p(x) := ((-1^m)/c) \prod_{k=1}^{m}(x - \lambda_k)$ with $c := \prod_{k=1}^{m} \lambda_k$ is in $\overline{\Pi}_m$ and with this p we have $p(\mathbf{A})\mathbf{e}_0 = \mathbf{0}$ and therefore $||p(\mathbf{A})\mathbf{e}_0||_{\mathbf{A}} = 0$ and thus, $\tilde{f}$ is minimal. □

5. The cg-algorithm as an iterative process

The cg-algorithm is ordinarily applied to large but sparse matrices. Therefore, one is not interested in carrying out all iteration steps. One is interested instead in an estimation of the magnitude of the error or the residual vector measured in some norm. The principal error estimations can be taken from (22) and (23) by applying $|| \quad ||_{\mathbf{A}}$ and using the definition (36) and (44) of Theorem 23 of the Appendix. We obtain

$$(26) \quad ||\mathbf{e}_j||_{\mathbf{A}} \le e_j||\mathbf{e}_0||_{\mathbf{A}}, \quad ||\mathbf{r}_j||_{\mathbf{A}} \le e_j||\mathbf{r}_0||_{\mathbf{A}}, \quad e_j := \min_{p \in \overline{\Pi}_j} \max_{\lambda \in \sigma(\mathbf{A})} |p(\lambda)|,$$

where $\overline{\Pi}_j$ is defined in (21). In order to obtain an estimate for e_j any polynomial $p \in \overline{\Pi}_j$ can be used. Let $I := [a, b]$ be a given interval with $0 < a < b$. Put $p(x) := ((-1)^j/c_j) \prod_{k=1}^{j}(x - x_k)$ with Chebyshev knots $x_k := \frac{1}{2}\{a + b + (b - a)\cos\big(\frac{2(j-k+1)-1}{2j}\pi\big)\}$, $k = 1, 2, \ldots, j$ in $[a, b]$ and $c_j := \prod_{k=1}^{j} x_k$. Then, $p \in \overline{\Pi}_j$ and $\max_{x \in [a,b]} |p(x)| = p(a)$. Now, $p(a) = \frac{(x_1-a)(x_2-a)\cdots(x_j-a)}{x_1 x_2 \cdots x_j} = \prod_{k=1}^{j}\big(1 - \frac{a}{x_k}\big) \le \big(1 - \frac{a}{b}\big)^j$. If we put $a := \lambda_{\min} := \min_{\lambda \in \sigma(\mathbf{A})} \lambda$ and $b := \lambda_{\max} := \max_{\lambda \in \sigma(\mathbf{A})} \lambda$ we obtain

$$(27) \qquad e_j \le \big(1 - d\big)^j, \quad d := \frac{\lambda_{\min}}{\lambda_{\max}}$$

which is sufficient to guarantee convergence since $0 < d \le 1$. However, this bound is the known bound for the steepest descent method and thus, not reflecting the true behavior of the cg-algorithm. According to Daniel, [1971, p. 121] we have

$$p(a) = \frac{2(1-d)^j}{(1+\sqrt{d})^{2j} + (1-\sqrt{d})^{2j}} < 2\Big(\frac{1-\sqrt{d}}{1+\sqrt{d}}\Big)^j, \quad d := \frac{\lambda_{\min}}{\lambda_{\max}}.$$

Therefore, we obtain

$$(28) \qquad e_j \le p(a) < 2\Big(\frac{1-\sqrt{d}}{1+\sqrt{d}}\Big)^j, \quad d := \frac{\lambda_{\min}}{\lambda_{\max}}.$$

We can also obtain estimates for $||\mathbf{e}||, ||\mathbf{r}||$ (rather than for $||\mathbf{e}||_{\mathbf{A}}, ||\mathbf{r}||_{\mathbf{A}}$) since there are positive constants $\mu \le M$ with

$$(29) \qquad \mu||\mathbf{x}|| \le ||\mathbf{x}||_{\mathbf{A}} \le M||\mathbf{x}|| \text{ for all } \mathbf{x}.$$

If we introduce an eigenvektor $\mathbf{x}$ of $\mathbf{A}$ into (29) we obtain $\mu||\mathbf{x}|| \le \sqrt{\lambda}||\mathbf{x}|| \le M||\mathbf{x}||$ and therefore, $\mu = \sqrt{\lambda_{\min}}$, $M = \sqrt{\lambda_{\max}}$ and from (26) we deduce

$$(30) \qquad ||\mathbf{e}_j|| \le \frac{e_j}{\sqrt{d}}||\mathbf{e}_0||, \quad ||\mathbf{r}_j|| \le \frac{e_j}{\sqrt{d}}||\mathbf{r}_0||, \quad d := \frac{\lambda_{\min}}{\lambda_{\max}}$$

where an estimation for e_j can be taken from (28). The derivations of this section could also be applied to generalizations of other offsprings of the cg-algorithm, like the FLETCHER-REEVES algorithm [1964]. A Hilbert space approach can be found in (LUENBERGER, [1969, Ch. 10.6]) where non commutativity is however not considered. The setting here would be as follows. As ground space take any Hilbert space H over the quaternions $\mathbb{H}$ where the scalar product must obey the formal rules given in (14). The matrix $\mathbf{A}$ has to be replaced by a linear, bounded, selfadjoint, positive definite operator A where linearity means here only $A(x+y) = Ax + Ay$ and $A(xc) = (Ax)c$ for all $x, y \in H$ and for all $c \in \mathbb{H}$. But this would lead to another topic.

6. An alternative approach via double sized complex matrices

There is a well known isomorphism between $\mathbb{H}$ and $\mathbb{C}^2$ (V. D. WAERDEN, [1960, p. 55]), where the multiplication $\mathbb{C}^2 \times \mathbb{C}^2 \to \mathbb{C}^2$ is arranged as follows: Let $(\alpha_j, \beta_j) \in \mathbb{C}^2$, define the two matrices

$$\mathbf{A}_j := \begin{pmatrix} \alpha_j & \beta_j \\ -\overline{\beta_j} & \overline{\alpha_j} \end{pmatrix}, \quad j = 1, 2 \tag{31}$$

and form the product $\mathbf{C} := \mathbf{A}_1 \mathbf{A}_2$. Then, the two entries of the first row of $\mathbf{C}$ define the product of the two given complex pairs. The correspondence between $\mathbb{H}$ and $\mathbb{C}^2$ is as follows. If $h := (a_1, a_2, a_3, a_4) \in \mathbb{H}$ then, $(\alpha, \beta) := (a_1 + \mathrm{i}a_2, a_3 + \mathrm{i}a_4) \in \mathbb{C}^2$ and vice versa. We call a complex (2×2) matrix of the form given in (31) a *complex* (2×2) *quaternion matrix*. A general complex $(2m \times 2n)$ matrix $\mathbf{A}$ will be called a *complex quaternion matrix* if all (2×2) submatrices $\begin{pmatrix} a_{2j-1,2k-1} & a_{2j-1,2k} \\ a_{2j,2k-1} & a_{2j,2k} \end{pmatrix}, j = 1, 2, \ldots m, \; k = 1, 2, \ldots, n$ are complex (2×2) quaternion matrices, where a_{jk} are the complex entries of $\mathbf{A}$. The following theorem is of importance here.

Theorem 12. Let $\mathbf{A} \in \mathbb{H}^{n \times n}$ be arbitrary and $\tilde{\mathbf{A}} \in \mathbb{C}^{2n \times 2n}$ the corresponding complex quaternion matrix. Then, the $2n$ eigenvalues of $\tilde{\mathbf{A}}$ form n pairs of complex conjugate numbers. In particular, all real eigenvalues are double. Hence, the number of non equivalent eigenvalues of $\mathbf{A}$ is at most n.

Proof: LEE, [1949]. □

Let $\mathbf{A}$ be an arbitrary matrix with quaternion entries. In order to distinguish between the four components of a specific entry a_{jk} we use the notation $a_{jk\ell}$ where $\ell = 1, 2, 3, 4$. Thus,

$$a_{jk} = a_{jk1}\mathrm{h} + a_{jk2}\mathrm{i} + a_{jk3}\mathrm{j} + a_{jk4}\mathrm{k}.$$

Similarly, the four entries of the components $\mathbf{x}_j$ of a quaternion-valued vector $\mathbf{x}$ are identified by $\mathbf{x}_{j1}, \mathbf{x}_{j2}, \mathbf{x}_{j3}, \mathbf{x}_{j4}$. Let $\mathbf{A}\mathbf{x} = \mathbf{b}$ be a linear square system with quaternion entries, $\mathbf{A} \in \mathbb{H}^{n\times n}, \mathbf{x}, \mathbf{b} \in \mathbb{H}^{n\times 1}$. We write the isomorphic system in complex quaternion matrices as $\tilde{\mathbf{A}}\tilde{\mathbf{x}} = \tilde{\mathbf{b}}$ where $\tilde{\mathbf{A}} \in \mathbb{C}^{2n\times 2n}, \tilde{\mathbf{x}}, \tilde{\mathbf{b}} \in \mathbb{C}^{2n\times 2}$. Then, $\tilde{\mathbf{x}}, \tilde{\mathbf{b}}$ have the form

$$\tilde{\mathbf{x}} =: (\,\boldsymbol{\xi} \quad \boldsymbol{\eta}\,) := \begin{pmatrix} x_{11} + \mathrm{i}x_{12} & x_{13} + \mathrm{i}x_{14} \\ -x_{13} + \mathrm{i}x_{14} & x_{11} - \mathrm{i}x_{12} \\ x_{21} + \mathrm{i}x_{22} & x_{23} + \mathrm{i}x_{24} \\ -x_{23} + \mathrm{i}x_{24} & x_{21} - \mathrm{i}x_{22} \\ \vdots & \vdots \\ x_{n1} + \mathrm{i}x_{n2} & x_{n3} + \mathrm{i}x_{n4} \\ -x_{n3} + \mathrm{i}x_{n4} & x_{n1} - \mathrm{i}x_{n2} \end{pmatrix}, \tag{32a}$$

$$\tilde{\mathbf{b}} =: (\,\boldsymbol{\beta} \quad \boldsymbol{\gamma}\,) := \begin{pmatrix} b_{11} + \mathrm{i}b_{12} & b_{13} + \mathrm{i}b_{14} \\ -b_{13} + \mathrm{i}b_{14} & b_{11} - \mathrm{i}b_{12} \\ b_{21} + \mathrm{i}b_{22} & b_{23} + \mathrm{i}b_{24} \\ -b_{23} + \mathrm{i}b_{24} & b_{21} - \mathrm{i}b_{22} \\ \vdots & \vdots \\ b_{n1} + \mathrm{i}b_{n2} & b_{n3} + \mathrm{i}b_{n4} \\ -b_{n3} + \mathrm{i}b_{n4} & b_{n1} - \mathrm{i}b_{n2} \end{pmatrix}. \tag{32b}$$

We see, that the second columns of $\tilde{\mathbf{x}}$ and of $\tilde{\mathbf{b}}$ are redundant. We delete these columns and treat the complex problem

$$\tilde{\mathbf{A}}\boldsymbol{\xi} = \boldsymbol{\beta} \tag{33}$$

with $\boldsymbol{\xi}, \boldsymbol{\beta}$ defined in (32). In order to obtain the final solution we have to replace ξ_{2j} with $-\overline{\xi_{2j}}$, $j = 1, 2, \ldots, n$ where $\boldsymbol{\xi} =: (\xi_1, \xi_2, \ldots, \xi_{2n})^{\mathrm{T}}$. In terms of quaternions the final solution $\mathbf{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ is

$$x_j = \Re\xi_{2j-1}\mathrm{h} + \Im\xi_{2j-1}\mathrm{i} - \Re\xi_{2j}\mathrm{j} + \Im\xi_{2j}\mathrm{k}, \quad j = 1, 2, \ldots, n. \tag{34}$$

If we compare the direct method using quaternions with the method described here using double sized complex matrices then, the operation count is the same. The essential work of the algorithm is in line `4`. In either case it is $32n^2$ (real) flops. Though the algebraic work is the same, the formulation via complex matrices may suffer from severe instabilities. There is a very simple example in Janovská & Opfer [2004] and also in the already mentioned paper by Dongarra et alii, [1984] there is a remark that quaternion algebra should be preferred.

7. The cg-algorithm for hermitean, indefinite matrices

For the real and complex case a thorough investigation of the case mentioned in the title was made by Modersitzki, [1995] where even more general matrices were considered. One of the main ingredients was a theorem by Faber & Manteuffel, [1984], which characterizes those matrices for which the cg-algorithm is possible. One of the results was that the spectrum of those matrices must be in a segment of $\mathbb{C}$. Since quaternion-valued matrices may have eigenvalues which are quaternions, it is not straightforward to generalize the theorem by Faber & Manteuffel. The only possibility for a break down of the cg-algorithm when positive definiteness is missing is in program line `5` where a division by zero cannot be excluded. However, if we look at indefinite, hermitean examples, we see the same behavior as in the real or complex case, namely that the cg-algorithm nevertheless works. A theoretical investigation of this case would need a thorough check of all results given and mentioned by Modersitzki. We leave this problem to another investigation.

8. Numerical Examples

We shall present three examples to show how the cg-algorithm applied to quaternion-valued matrices behaves. All matrices employed are hermitean, but not necessarily positive definite. The positive definite matrices $\mathbf{A}$ were constructed according to $\mathbf{A} = \mathbf{B}^*\mathbf{B}$, the hermitean matrices $\mathbf{A}$ were constructed according to $\mathbf{A} = \mathbf{B}^* + \mathbf{B}$. The quaternion-valued matrices $\mathbf{B}$ were filled at all positions with uniformly distributed random integers in $[-5, 5]$. Thus, the employed matrices $\mathbf{A}$ also have integer entries and are therefore, exact hermitean matrices. For the demonstration we always sketched the development of the residual and the true error in dependence of the iteration number. In order to know the true error, the right hand side was always maneuvered in such a way that the solution was known a priori. In the first two examples, the matrices are full (200×200) quaternion-valued matrices. In the first case all 200 eigenvalues are positive, where in the second case the number of negative and positive eigenvalues is about the same. In the third example, $\mathbf{A}$ is a (200×200) diagonal matrix with 100 double eigenvalues $-9\mathrm{h}, -7\mathrm{h}, -5\mathrm{h}, \ldots, 189\mathrm{h}$ where h is defined in (5). An analog matrix, however with single (real) eigenvalues was used by PAIGE, PARLETT, & VAN DER VORST, [1995].

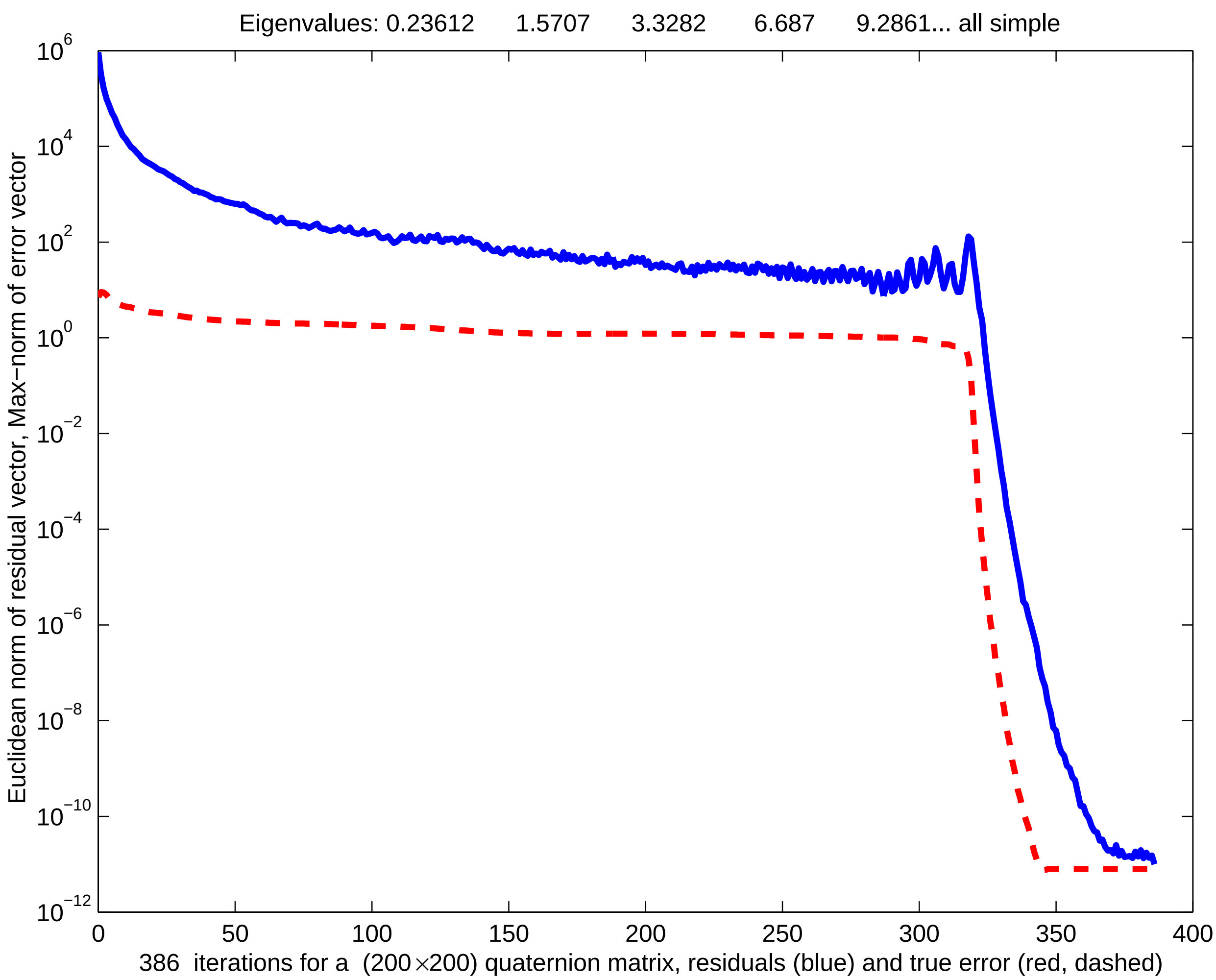

Figure13. Residuum (solid) and true error (dashed) of cg-algorithm applied to a (200×200) hermitean, positive definite matrix

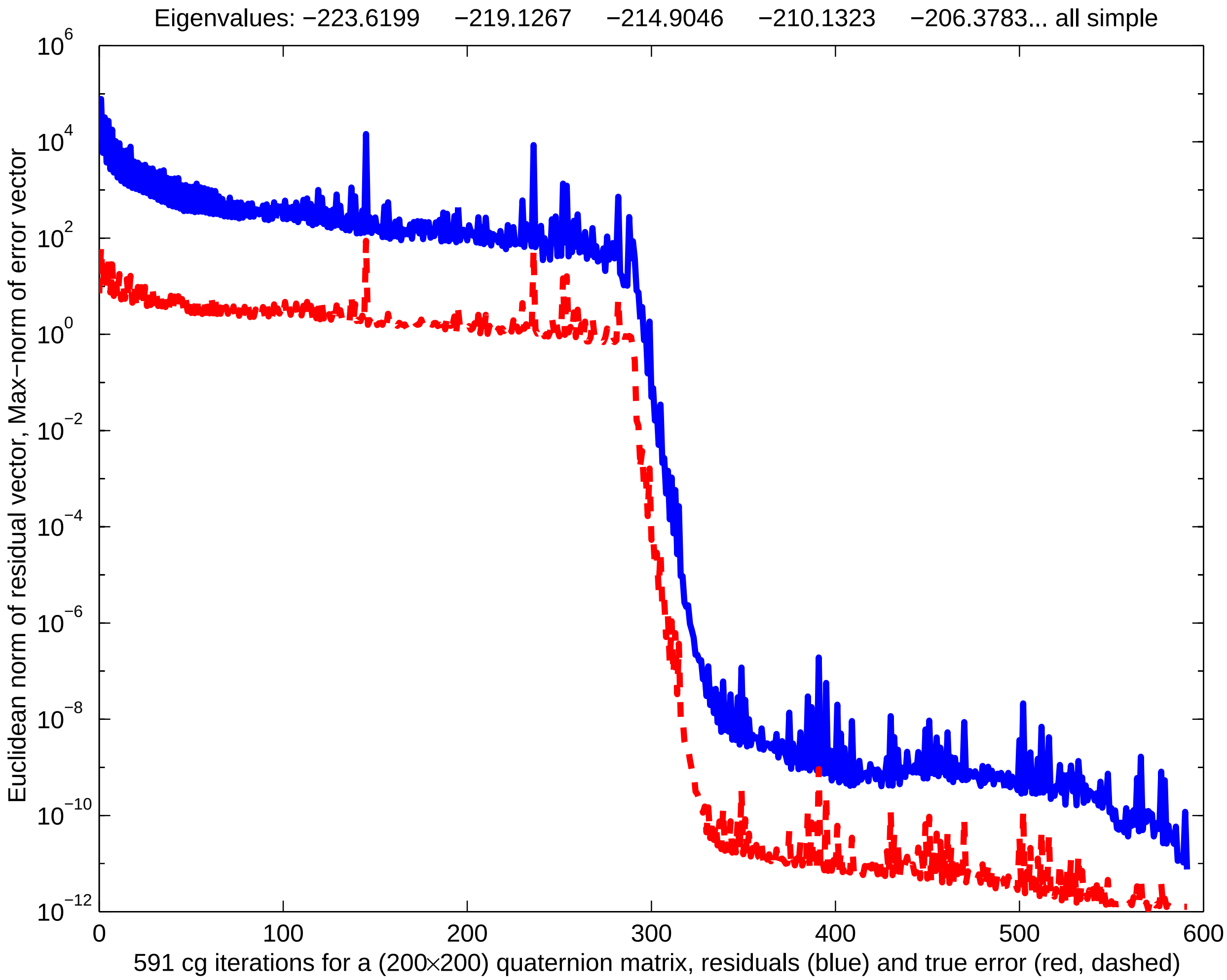

Figure14. Residuum (solid) and true error (dashed) of cg-algorithm applied to a (200×200) hermitean, but indefinite matrix

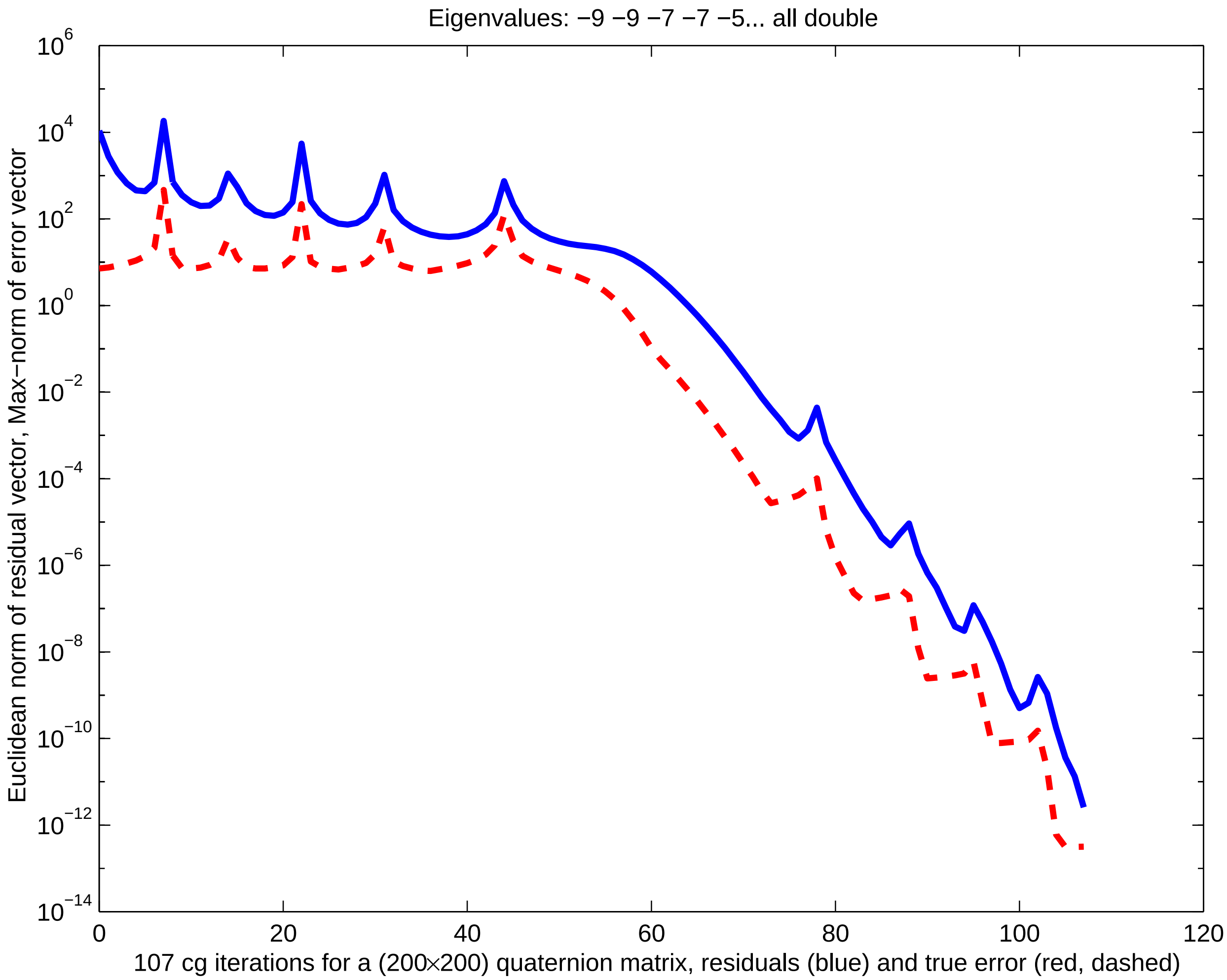

Figure15. Residuum (solid) and true error (dashed) of cg-algorithm applied to a (200×200) hermitean, but indefinite diagonal matrix with all eigenvalues double

We see in the indefinite case that the residuum is more likely to oscillate and that in that case the cg-algorithm needs more steps than in the corresponding definite case. In the last case (Figure 15) we can very well see the influence of the 5 (double) negative eigenvalues. See the comments in the real case by Fischer, [1996, pp. 167–170].

A closer look at Program 2 reveals the following flop counts per iteration:

Line `4`. Matrix∗Vector: $32n^2$,
Line `5`. Scalar product, Real division: $32n + 1$,
Line `6`. Real∗Vector, Vector+Vector: $8n$,
Line `7`. Real∗Vector, Vector+Vector: $8n$,
Line `8`. Scalar product: $32n$,
Line `9`. Real Division: 1,
Line `10`. Real∗Vector, Vector+Vector: $8n$.

The sum of it is

$$cpl_{\text{cg}} := 32n^2 + 88n + 2. \tag{35}$$

That means, that the creation of the matrix $\mathbf{A} := \mathbf{B}^*\mathbf{B}$ is roughly of the same magnitude as finding the solution of $\mathbf{Ax} = \mathbf{b}$ by the cg-algorithm when magnitude is measured by flop counts.

9. Appendix: The determination of $||p(\mathbf{A})||_\mathbf{A}$

The results of this section have been used to derive error estimates in Section 5. Let $\mathbf{A}$ be hermitean and positive definite. If $\mathbf{B} \in \mathbb{H}^{n\times n}$ is arbitrary, then, we can define the *operator norm*

$$||\mathbf{B}||_\mathbf{A} := \sup_{\mathbf{x}\neq\mathbf{0}} \frac{||\mathbf{Bx}||_\mathbf{A}}{||\mathbf{x}||_\mathbf{A}}, \tag{36}$$

also for quaternion-valued matrices with the consequence, that

$$||\mathbf{Bx}||_\mathbf{A} \le ||\mathbf{B}||_\mathbf{A}||\mathbf{x}||_\mathbf{A} \text{ for all } \mathbf{x} \in \mathbb{H}^n. \tag{37}$$

We shall need a lemma which says that under a certain condition even several matrices can be diagonalized by the same orthogonal matrix.

Lemma 16. Let $\mathcal{F}$ be a family of normal matrices of the same order with quaternion entries. Then, there is a single orthogonal matrix $\mathbf{U}$ such that $\mathbf{U}^*\mathbf{F}\mathbf{U}$ is a diagonal matrix for each $\mathbf{F} \in \mathcal{F}$ if and only if all pairs in $\mathcal{F}$ commute.

Proof: Wiegmann, [1955].

Another reminder seems to be necessary. An arbitrary matrix $\mathbf{B} \in \mathbb{H}^{m\times n}$ is said to have *rank* r if r is the *right* column rank of $\mathbf{B}$, i. e. the maximum number of right independent columns.

Lemma 17. Let $\mathbf{B} \in \mathbb{H}^{n\times n}$. Then, $\mathbf{B}$ is non singular, if and only if the rank of $\mathbf{B}$ is n.

Proof: Zhang, [1997, p. 43].

It is possible that a matrix of rank r has a different *left* column rank. Thus, it is possible, that an invertible matrix $\mathbf{B}$ has a non invertible transpose $\mathbf{B}^{\mathrm{T}}$. A very simple example is (Zhang, [1997, p. 45]),

$$\mathbf{B} := \begin{pmatrix} \mathrm{h} & \mathrm{i} \\ \mathrm{j} & \mathrm{k} \end{pmatrix}, \quad \mathbf{B}^{-1} = \frac{1}{2}\begin{pmatrix} \mathrm{h} & -\mathrm{j} \\ -\mathrm{i} & -\mathrm{k} \end{pmatrix}. \tag{38}$$

The left column rank of this matrix $\mathbf{B}$ is only one, thus, $\mathbf{B}^{\mathrm{T}}$ is not invertible. We will need the following simple lemma.

Lemma 18. Let $\mathbf{A}, \mathbf{B} \in \mathbb{H}^{n\times n}$ be two upper triangular matrices with quaternion entries. (a) Then, the product $\mathbf{C} := \mathbf{AB}$ is again an upper triangular matrix and the diagonal entries c_{jj} of $\mathbf{C}$ are $c_{jj} = a_{jj}b_{jj}$ where a_{jj}, b_{jj} are the corresponding diagonal elements of $\mathbf{A}, \mathbf{B}$, respectively. (b) Let p be any polynomial, possibly with quaternion coefficients. Then, $p(\mathbf{A})$ is an upper triangular matrix with diagonal entries $p(a_{jj})$.

Proof: Let us denote the entries of $\mathbf{A}, \mathbf{B}, \mathbf{C}$ by a_{jk}, b_{jk}, c_{jk}, respectively. By assumption, $a_{jk} = b_{jk} = 0$ for $j > k$. Hence, (a) $c_{jj} = \sum_{k=1}^{n} a_{jk}b_{kj} = a_{jj}b_{jj}$. For $j > k$ we have $c_{jk} = \sum_{\ell=1}^{n} a_{j\ell}b_{\ell k} = \sum_{j\le\ell\le k} a_{j\ell}b_{\ell k} = 0$. (b) From (a) we know that $\mathbf{A}^2$ is an upper triangular matrix with $\mathrm{diag}(\mathbf{A}^2) = \mathrm{diag}(a_{11}^2, a_{22}^2, \ldots, a_{nn}^2)$. By induction it follows that $\mathbf{A}^j$ is upper triangular and $\mathrm{diag}(\mathbf{A}^j) = \mathrm{diag}(a_{11}^j, a_{22}^j, \ldots, a_{nn}^j)$ for all $j \ge 1$. Thus, $p(\mathbf{A})$ is also upper triangular and $\mathrm{diag}(p(\mathbf{A})) = p(\mathrm{diag}(\mathbf{A})) = \mathrm{diag}(p(a_{11}), p(a_{22}), \ldots, p(a_{nn}))$. □

Lemma 19. Let $\mathbf{B} \in \mathbb{H}^{n\times n}$ be an arbitrary matrix with spectrum $\sigma(\mathbf{B})$. Let p be an arbitrary polynomial with real coefficients. Then

$$\sigma(p(\mathbf{B})) = p(\sigma(\mathbf{B})) := \{p(\lambda) : \lambda \in \sigma(\mathbf{B})\}. \tag{39}$$

Proof: Let $\lambda \in \sigma(\mathbf{B})$. I. e. there is a vector $\mathbf{x} \neq \mathbf{0}$ with $\mathbf{Bx} = \mathbf{x}\lambda$. Therefore, $\mathbf{B}^{j+1}\mathbf{x} = \mathbf{B}^j\mathbf{B}\mathbf{x} = \mathbf{B}^j\mathbf{x}\lambda = \mathbf{x}\lambda^{j+1}$. Let $p(z) := \sum_{j=0}^m \alpha_j z^j$. Then, $p(\mathbf{B})\mathbf{x} := \sum_j^m \alpha_j \mathbf{B}^j\mathbf{x} = \sum_{j=0}^m \alpha_j \mathbf{x}\lambda^j = \mathbf{x}p(\lambda)$, since the α_j are real, hence, $p(\sigma(\mathbf{B})) \subset \sigma(p(\mathbf{B}))$. We have to show, that $p(\mathbf{B})$ has no other eigenvalues than those in $p(\sigma(\mathbf{B}))$. In order to show that, we use that there exists a Schur canonical form (Zhang, [1997], Wiegmann, [1955]) for $\mathbf{B}$. I. e. there exists an orthogonal matrix $\mathbf{U}$ such that $\Delta := \mathbf{U}^*\mathbf{B}\mathbf{U}$ is an upper triangular matrix where the diagonal elements are either real or complex with positive imaginary part. If we apply the polynomial p we obtain $p(\Delta) = p(\mathbf{U}^*\mathbf{B}\mathbf{U}) = \sum_{j=0}^m \alpha_j (\mathbf{U}^*\mathbf{B}\mathbf{U})^j = \sum_{j=0}^m \alpha_j \underbrace{\mathbf{U}^*\mathbf{B}\mathbf{U}\mathbf{U}^*\mathbf{B}\mathbf{U}\cdots\mathbf{U}^*\mathbf{B}\mathbf{U}}_{j \text{ times}} = \sum_{j=0}^m \alpha_j \mathbf{U}^*\mathbf{B}^j\mathbf{U}$ $= \mathbf{U}^*p(\mathbf{B})\mathbf{U}$ since the real coefficients α_j commute with quaternions. Thus, the matrices $p(\Delta)$ and $p(\mathbf{B})$ are similar and have therefore the same spectrum. According to Lemma 18, part (b) the matrix $p(\Delta)$ is upper triangular with diagonal elements $p(\delta_{jj})$ where δ_{jj} are the diagonal elements of Δ. However, according to the theorem of Schur the diagonal elements of Δ are the eigenvalues of $\mathbf{B}$. □

It should be remarked here, that for the proof any other triangular canonical form for $\mathbf{B}$ like the Jordan canonical would have worked. There exists such a Jordan canonical form, too (Wiegmann, [1955][1)]).

Example 20. Let $\mathbf{B} \in \mathbb{H}^{2\times 2}$ be the matrix defined in (38). Some computations reveal that (approximately) $\sigma(\mathbf{B}) = \{-0.3660 + 1.3660\mathrm{i},\ 1.3660 + 0.3660\mathrm{i}\}$. Let us define $p(x) := \mathrm{i}x$, then, $p(\mathbf{B}) = \begin{pmatrix} \mathrm{i} & -\mathrm{h} \\ \mathrm{k} & -\mathrm{j} \end{pmatrix}$ and $\sigma(p(\mathbf{B})) = \{-0.7071 + 1.2247\mathrm{i}, 0.7071 + 1.2247\mathrm{i}\}$[2)]. Now, it is easy to see, that $p(\sigma(\mathbf{B})) \neq \sigma(p(\mathbf{B}))$ since $p(\sigma(\mathbf{B})) = \mathrm{i}\sigma(\mathbf{B}) = \{-1.3660 - 0.3660\mathrm{i}, -0.3660 + 1.3660\mathrm{i}\}$. Thus, equation (39) will not be true in general if we permit polynomials p with non real coefficients.

Lemma 21. Let $\mathbf{A}, \mathbf{B} \in \mathbb{H}^{n\times n}$ where $\mathbf{A}$ is hermitean and positive definite and $\mathbf{B}$ is normal. Let the set of eigenvalues of $\mathbf{A}$ be denoted by

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[1)] According to Zhang & Wei, [2001], Wiegmann's proof is false, however, the statement remains true.

[2)] The eigenvalues of $\mathbf{B}$ are $\lambda_1 = (-a + \mathrm{i}b), \lambda_2 = (b + \mathrm{i}a)$ those of $\mathrm{i}\mathbf{B}$ are $\tilde{\lambda}_1 = (-\tilde{a} + \mathrm{i}\tilde{b}), \tilde{\lambda}_2 = (\tilde{a} + \mathrm{i}\tilde{b})$ with $a = 0.5(\sqrt{3} - 1), b = 0.5(\sqrt{3} + 1)$, $\tilde{a} = \sqrt{0.5}, \tilde{b} = \sqrt{1.5}$.

$\sigma(\mathbf{A}) := \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ and that of $\mathbf{B}$ by $\sigma(\mathbf{B}) := \{\mu_1, \mu_2, \ldots, \mu_n\}$. If $\mathbf{A}, \mathbf{B}$ commute then

$$||\mathbf{B}||_{\mathbf{A}} = \max_{\mu \in \sigma(\mathbf{B})} |\mu|. \tag{40}$$

Proof: Since $\mathbf{A}$ is also normal there is according to Lemma 16 (applied to a family consisting of $\mathbf{A}$ and $\mathbf{B}$) an orthogonal matrix $\mathbf{U}$ such that

$$\mathbf{AU} = \mathbf{UD_A}, \quad \mathbf{BU} = \mathbf{UD_B}, \text{ where} \tag{41a}$$

$$\mathbf{D_A} := \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n), \quad \mathbf{D_B} := \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_n). \tag{41b}$$

According to the definitions (15), (36) of $||\mathbf{B}||_{\mathbf{A}}$ we have

$$||\mathbf{B}||_{\mathbf{A}} := \sup_{\mathbf{x} \neq \mathbf{0}} \frac{||\mathbf{Bx}||_{\mathbf{A}}}{||\mathbf{x}||_{\mathbf{A}}} = \max_{||\mathbf{x}||_{\mathbf{A}}=1} ||\mathbf{Bx}||_{\mathbf{A}} = \max_{\mathbf{x}^*\mathbf{Ax}=1} \sqrt{\mathbf{x}^*\mathbf{B}^*\mathbf{ABx}}. \tag{42}$$

Now, $\mathbf{x}$ may be represented by $\mathbf{x} = \sum_j \mathbf{u}_j \beta_j$, where $\mathbf{u}_j$ are the columns of $\mathbf{U}$ and β_j are uniquely determined quaternions. Multiplying $\mathbf{x}$ (from the left) by $\mathbf{A}$ yields $\mathbf{Ax} = \sum_j \mathbf{Au}_j \beta_j = \sum_j \lambda_j \mathbf{u}_j \beta_j$, and multiplication by $\mathbf{B}$ yields $\mathbf{Bx} = \sum_j \mathbf{Bu}_j \beta_j = \sum_j \mathbf{u}_j \mu_j \beta_j$ where (41) was used and the fact that the λ_j are real. If we use the orthogonality of $\mathbf{U}$ we obtain from (42)

$$||\mathbf{B}||_{\mathbf{A}} = \max_{\sum_j \lambda_j |\beta_j|^2 = 1} \sqrt{\sum_j \lambda_j |\mu_j|^2 |\beta_j|^2}.$$

Put $c_j := \lambda_j |\beta_j|^2$, then, all $c_j \geq 0$ and because of $\lambda_j \neq 0$ for all j we have a 1-1 relation between the c_j and the $|\beta_j|$. Thus, we obtain

$$||\mathbf{B}||_{\mathbf{A}} = \max_{c_j \geq 0, \sum_j c_j = 1} \sqrt{\sum_j c_j |\mu_j|^2} = \max_j |\mu_j|,$$

since we are maximizing over all convex combinations of $|\mu_1|^2, |\mu_2|^2, \ldots, |\mu_n|^2$ and the $|\mu_j|$ are real. $\square$

We can not do without the commutativity in Lemma 18. This will be shown by the following example.

Example 22. Define the following two matrices

$$\mathbf{A} := \begin{pmatrix} 3 & a \\ \overline{a} & 3 \end{pmatrix}, \quad \mathbf{B} := \begin{pmatrix} 3 & a \\ \overline{a} & -3 \end{pmatrix}, \quad a := (1,1,1,1). \tag{43}$$

Both are hermitean and $\mathbf{A}$ is positive definite. They do not commute. We have $\sigma(\mathbf{A}) = \{1,5\}$, $\sigma(\mathbf{B}) = \{-\sqrt{13}, \sqrt{13}\}$. The matrix $\mathbf{A}$ has corresponding eigenvectors $\mathbf{u}_1 := (2, -\overline{a})^{\mathrm{T}}$, $\mathbf{u}_2 := (2, \overline{a})^{\mathrm{T}}$, and the matrix $\mathbf{B}$ has corresponding eigenvectors $\mathbf{v}_1 := (\sqrt{13} + 3, \overline{a})^{\mathrm{T}}$, $\mathbf{v}_2 := (\sqrt{13} - 3, -\overline{a})^{\mathrm{T}}$. Formula (40) would yield $||\mathbf{B}||_{\mathbf{A}} = \sqrt{13}$. However, if we put $\mathbf{x} := ((-1,-1,-1,0.6),(1,0.6,-0.6,-0.6))^{\mathrm{T}}$, then, $\sqrt{\frac{\mathbf{x}^*\mathbf{B}^*\mathbf{A}\mathbf{B}\mathbf{x}}{\mathbf{x}^*\mathbf{A}\mathbf{x}}} = \sqrt{154/3}$ which is larger than $\sqrt{13}$.

Theorem 23. Let $\mathbf{A} \in \mathbb{H}^{n\times n}$ be a hermitean, positive definite matrix, $\sigma(\mathbf{A})$ its spectrum and p any polynomial with real coefficients. Then

$$||p(\mathbf{A})||_{\mathbf{A}} = \max_{\lambda\in\sigma(\mathbf{A})} |p(\lambda)|, \tag{44}$$

where the operator norm $||\quad||_{\mathbf{A}}$ is defined in (36).

Proof: Since $p(\mathbf{A})$ is hermitean und thus, normal and since $\mathbf{A}$ and $p(\mathbf{A})$ commute for all polynomials p with real coefficients, we can apply formula (40) of the above Lemma 21 which yields $||p(\mathbf{A})||_{\mathbf{A}} = \max_{\mu\in\sigma(p(\mathbf{A}))} |\mu|$. A final application of formula (39) of Lemma 19 to the right hand side yields the desired result (44). □

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