Quaternions and quaternionic polynomials

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Motivation: Quantum Mechanics

Quantum Mechanics

Electronic structure of molecules and solids that contain heavy atoms
$\Longrightarrow$ the use of relativistic kinematics is required

- effects that do not change the symmetry of the problem (mass-velocity terms, Darwin terms...)
- effects that modify symmetry (spin-orbit coupling)

Computation

- without spin-orbit:
  matrix elements $\in \langle 10^{-5}, 1\rangle$,
  the smallest eigenvalue $\sim 10^{-9}$
- inclusion of spin-orbit coupling:
  matrix is doubled in size and becomes complex $\Rightarrow$ the numerical noise will dramatically increase,
  the smallest eigenvalue occurs twice,
  classical techniques cannot be used directly.

J.J.Dongarra, J.R.Gabriel, D.D.Koelling, J.H.Wilkinson: *Solving the Secular Equation Including Spin Orbit Coupling for Systems with Inversion and Time Reversal Symmetry*, J. Comput. Phys., **54** (1984), 278–288.

without spin orbit		spin-orbit effects included
$a \in \mathbb{R}$	$\longrightarrow$	$\begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}$
scalar matrix element		2×2 matrix with complex elements

$$h = (a_1, a_2, a_3, a_4) \in \mathbb{H}$$

$$\widetilde{h} = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}, \ \alpha = a_1 + i\, a_2, \ \beta = a_3 + i\, a_4, \ \widetilde{h} \in \widetilde{\mathbb{H}}$$

$\mathbb{H}$ and $\widetilde{\mathbb{H}}$ are isomorphic

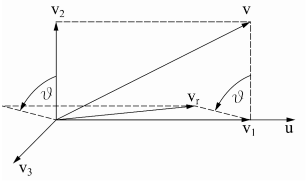
quaternion arithmetic?

-increased accuracy
-economy of storage
$\times$ more computational effort

B. L. van der Waerden: *Algebra I, 5. Aufl.*, Springer, Berlin, 1960 (1st ed. 1936)

Rotation of vectors

Quaternions can be used to represent many operations in 3-D space, including rotations, affine transformations and projections:



The rotation of the vector $\mathbf{v}$ about the vector $\mathbf{u}$ ($\|\mathbf{u}\| = 1$) by the angle θ:

$$\mathbf{v_1} = (\mathbf{u}\cdot\mathbf{v})\mathbf{u} \quad \ldots \quad \text{the projection of } \mathbf{v} \text{ onto } \mathbf{u}$$

$$\mathbf{v_3} = \mathbf{v} - (\mathbf{u}\cdot\mathbf{v})\mathbf{u} \quad \ldots \quad \text{component of } \mathbf{v} \text{ orthogonal to } \mathbf{u}$$

$$\mathbf{v_2} = \mathbf{u}\times\mathbf{v} \quad \longrightarrow \quad \mathbf{v_r} = \mathbf{v_1} + \cos\vartheta\, \mathbf{v_2} + \sin\vartheta\, \mathbf{v_3}$$

Thus, $\mathbf{v_r} = (\mathbf{u}\cdot\mathbf{v})\mathbf{u} + \cos\vartheta\,(\mathbf{v} - (\mathbf{u}\cdot\mathbf{v})\mathbf{u}) + \sin\vartheta\,(\mathbf{u}\times\mathbf{v})\,.$

Via quaternions:

$$p = (0, \mathbf{v}), \quad q = \left(\cos\frac{\vartheta}{2}, \mathbf{u}\sin\frac{\vartheta}{2}\right) \quad \Longrightarrow \quad p_r = q\,p\,q^{-1} = (0, \mathbf{v_r})\,.$$

Broombridge, Dublin

Here as he walked by
on the 16th of October 1843
Sir William Rowan Hamilton
in a flash of genius discovered
the fundamental formula for
quaternion multiplication
$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = \mathbf{ijk} = -1$
& cut it on a stone of this bridge.

Idea: Numerical Linear Algebra for Quaternions

- Janovská D., Opfer G.: Givens' transformation applied to quaternion valued vectors, BIT Numerical Mathematics 43, No.5 (2003), 991 – 1002.
- Janovská D., Opfer G.: Givens transformation for quaternion-valued matrices applied to Hessenberg reduction, ETNA, Electronic Transactions on Numerical Analysis, Vol.20, 2005, pp.1 – 26.
- Janovská D., Opfer G.: Computing quaternionic roots by Newton's method, Electronic Transactions on Numerical Analysis (ETNA), Vol.26 (2007), pp.82 – 102.
- Janovská D., Opfer G.: Linear Quaternionic Systems, Mitt. Math. Ges. Hamburg 27 (2008), 223 – 234.
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- Janovská D., Opfer G.: A note on the computation of all zeros of simple quaternionic polynomials, SIAM J. Numer. Anal. 48 (2010), 244 – 256.
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- Janovská D., Opfer G.: The Nonexistence of Pseudoquaternions in $\mathbb{C}^{2\times 2}$, Advances in Applied Clifford Algebras 21 (2011), 531 – 540.

Basic definitions for quaternions

Let $\mathbb{H} := \mathbb{R}^4$ be the skew field of quaternions

Let $x = (x_1, x_2, x_3, x_4), \quad y = (y_1, y_2, y_3, y_4) \in \mathbb{H}$.

- The first component x_1 ... the real part of x, denoted by $\Re x$.
- $\mathbf{v} = (x_2, x_3, x_4) \in \mathbb{R}^3$ ... the vector part of x
- The second component x_2 ... the imaginary part of x, denoted by $\Im x$.
- $x = (x_1, 0, 0, 0)$ will be identified with $x_1 \in \mathbb{R}$
- $x = (x_1, x_2, 0, 0)$ will be identified with $x_1 + \mathrm{i}x_2 \in \mathbb{C}$
- The conjugate of x will be defined by $\overline{x} = (x_1, -x_2, -x_3, -x_4)$
- The absolute value of x will be defined by $|x| = \sqrt{x_1^2 + x_2^2 + x_3^2 + x_4^2}$
- The inverse quaternion is defined as $x^{-1} = \dfrac{\overline{x}}{|x|^2}$ for $x \in \mathbb{H}\backslash\{0\}$
- Four basis elements of $\mathbb{H}$:
  $\mathbf{1} = (1, 0, 0, 0),\ \mathbf{i} = (0, 1, 0, 0),\ \mathbf{j} = (0, 0, 1, 0),\ \mathbf{k} = (0, 0, 0, 1),$

Let $x = (x_1, x_2, x_3, x_4)$, $\quad y = (y_1, y_2, y_3, y_4) \in \mathbb{H}$. Then

$$x + y = (x_1 + y_1, x_2 + y_2, x_3 + y_3, x_4 + y_4)\,.$$

Let $x = (x_1, x_2, x_3, x_4) \in \mathbb{H}$, x can be represented as
$x = x_1 + x_2\,\mathbf{i} + x_3\,\mathbf{j} + x_4\,\mathbf{k}$ or as $x = (x_1, \mathbf{v})\,,\ x_1 \in \mathbb{R}\,,\ \mathbf{v} = (x_2, x_3, x_4) \in \mathbb{R}^3\,.$

$\mathbb{H}$ has the ordinary vector space structure with an additional multiplicative operation $\mathbb{H} \times \mathbb{H} \longrightarrow \mathbb{H}$ defined by a multiplication table for the basis elements:

	1	**i**	**j**	**k**
1	**1**	**i**	**j**	**k**
i	**i**	−**1**	**k**	−**j**
j	**j**	−**k**	−**1**	**i**
k	**k**	**j**	−**i**	−**1**

(1)

In general, multiplication is not commutative here, but there are some classes of quaternions for which the product commutes (for example if one of the factors is real).

The multiplication rule: $x = (x_1, x_2, x_3, x_4),\ y = (y_1, y_2, y_3, y_4) \in \mathbb{H}$, then

$$\begin{aligned} xy \quad = \quad & (x_1y_1 - x_2y_2 - x_3y_3 - x_4y_4,\ x_1y_2 + x_2y_1 + x_3y_4 - x_4y_3, \\ & x_1y_3 - x_2y_4 + x_3y_1 + x_4y_2,\ x_1y_4 + x_2y_3 - x_3y_2 + x_4y_1) \end{aligned}$$

(16 multiplications and 12 additions of real numbers).

The multiplication rule implies

$$\Re(xy) = \Re(yx)\,, \quad \alpha x = x\alpha \quad \text{for} \quad x, y \in \mathbb{H},\ \alpha \in \mathbb{R}\,. \tag{2}$$

Remark If we represent quaternions x and y as $x = (x_1, \mathbf{v}_1),\ y = (y_1, \mathbf{v}_2)$, $x_1, y_1 \in \mathbb{R},\ \mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^3$ then we have

$$xy = (x_1y_1 - \mathbf{v}_1 \cdot \mathbf{v}_2,\ x_1\mathbf{v}_2 + y_1\mathbf{v}_1 + \mathbf{v}_1 \times \mathbf{v}_2)$$

($\cdot$ means a scalar, $\times$ means a vector product in $\mathbb{R}^3$).

Classes of equivalence

Two quaternions x and y are called equivalent, $\mathbf{x} \sim \mathbf{y}$, if there is $h \in \mathbb{H}\backslash\{0\}$ such that $y = h^{-1}xh$. Then we denote $[x]$ an equivalence class of the quaternion x,

$$[x] = \{y \in \mathbb{H} : \; y = h^{-1}xh \; \text{ for all } \; h \in \mathbb{H}\backslash\{0\}\}.$$

Lemma Two quaternions x and y are equivalent if and only if

$$\Re x = \Re y \quad \text{and} \quad |x| = |y|. \tag{3}$$

Proof.

(a) Let $x \sim y$, i.e., $y = \alpha^{-1}x\alpha$ or $\alpha y = x\alpha$ for some $\alpha \in \mathbb{H}\backslash\{0\}$.

Then $|\alpha y| = |x\alpha| \implies |\alpha||y| = |x||\alpha| \implies |x| = |y|$.

The formula (2) implies that
$\Re y = \Re\left(\alpha^{-1}x\alpha\right) = \Re\left(x\alpha\,\alpha^{-1}\right) = \Re x$.

(b) Let $\Re x = \Re y$ and $|x| = |y|$ for two quaternions x, y. We have to show that there is an $\alpha \in \mathbb{H}\backslash\{0\}$ such that $y = \alpha^{-1} x \alpha$, i.e., $\alpha y = x \alpha$.

Let us set

$$u = y - x = (u_1, u_2, u_3, u_4), \; v = y + x = (v_1, v_2, v_3, v_4), \; \alpha = (\alpha_1, \alpha_2, \alpha_3, \alpha_4).$$

Because $\Re x = \Re y$, we have $u_1 = 0$. Then $\alpha y = x \alpha$ is equivalent to the homogeneous real 4×4 system

$$\mathbf{M}\alpha = \mathbf{0}, \qquad \text{where} \qquad \mathbf{M} = \begin{pmatrix} 0 & -u_2 & -u_3 & -u_4 \\ u_2 & 0 & v_4 & -v_3 \\ u_3 & -v_4 & 0 & v_2 \\ u_4 & v_3 & -v_2 & 0 \end{pmatrix}.$$

We have to show that **M** is singular under the condition $|x| = |y|$, i.e., under the condition $u_2 v_2 + u_3 v_3 + u_4 v_4 = 0$.

The expansion of **M** with respect to the first column reveals that under this condition all four summands in $\det \mathbf{M}$ vanish, thus **M** is singular and $\alpha y = x \alpha$ has a nontrivial solution α.

□

Corollary. Let $x = (x_1, x_2, x_3, x_4)$. Then the equivalence class $[x]$ contains exactly two complex numbers a and $\overline{a}$, where

$$a = (x_1, \sqrt{x_2^2 + x_3^2 + x_4^2}, 0, 0) = x_1 + |x_v|\,\mathbf{i} \in [x]\,,$$

i.e., a is the only complex element in $[x]$ with non negative imaginary part.

$a \ldots$ the complex representative of $[x]$.

Remark

If a is real then $[a] = \{a\}$, i.e. $[a]$ contains only one element $\{a\}$

If a is not real, then $[a]$ always contains infinitely many elements,

$$[a] = \{z \in \mathbb{H},\ \Re z = \Re a,\ |z| = |a|\}\,, \quad \ldots \quad \text{the surface of a ball in } \mathbb{R}^3\,.$$

Simple quaternionic polynomials

Let $p_n(z)$ be a given quaternionic polynomial of degree n,

$$p_n(z) = \sum_{j=0}^{n} a_j z^j \,, \quad z,\, a_j \in \mathbb{H},\, j = 0, 1, 2, \ldots, n, \quad a_0,\, a_n \neq 0 \,, \tag{4}$$

$a_0 \neq 0$ ... the origin is never a zero of p_n
$a_n \neq 0$ ... polynomial degree is not less then n
$p_n(z)$ ... one-sided (or simple) quaternionic polynomial.

In general, if a zero z_0 of a quaternionic polynomial is real, then $h^{-1}z_0h = z_0h^{-1}h = z_0$, and the real zero is the only zero of this quaternionic polynomial.

Example Let $p_2(z) = z^2 + 1$ ... zeros $\pm\mathbf{i}$.
So, there is the only one class of zeros, the complex representative is $+\mathbf{i}$. All zeros have the form $h^{-1}(\pm\mathbf{i})h$ for all $h \in \mathbb{H},\ h \neq 0$.

This polynomial as the quaternionic one sided polynomial has infinitely many quaternionic zeros.

Isolated and spherical zeros

Definition Let z_0 be a zero of p_n. If z_0 is not real and it has the property

$$p_n(z) = 0 \text{ for all } z \in [z_0]$$

we say that z_0 generates a spherical zero or is a spherical zero.

If z_0 is real or does not generate a spherical zero, it is called an isolated zero.

Remarks

- z_0 a zero of p_n ... all elements of $[z_0]$ are zeros or only z_0 is zero
- two zeros $\pm\mathbf{i}$ of $p_2(z) = z^2 + 1$ generate the same spherical zero
- More generally, all non real zeros of polynomials with real coefficients are spherical zeros
- Real zeros of any polynomial are always isolated zeros
- Eilenberg and Niven, 1944: There exists at least one zero
- Pogorui and Shapiro, 2004: The number of both types of zeros together does not exceed n (all spherical zeroes of the same equivalence class count as one zero)

All powers of a quaternion

Iteration process (two term recursion):

$$\begin{aligned} z^j &= \alpha_j z + \beta_j, \quad \alpha_j, \beta_j \in \mathbb{R}, \quad j = 0, 1, \ldots, \text{ where} \qquad (5) \\ \alpha_0 &= 0, \quad \beta_0 = 1, \\ \alpha_{j+1} &= 2\Re z\, \alpha_j + \beta_j, \\ \beta_{j+1} &= -|z|^2 \alpha_j, \quad j = 0, 1, \ldots \end{aligned}$$

In order to compute all powers of $z \in \mathbb{H}$ up to degree n, one needs $n - 1$ quaternionic multiplications (one quaternionic multiplication = 28 flops), whereas the recursion needs only $3n$ flops.

Example Let us compute $z^2 = \alpha_2 z + \beta_2$.

$$\alpha_0 = 0, \; \beta_0 = 1, \; \alpha_1 = \beta_0 = 1, \; \beta_1 = -|z|^2 \alpha_0 = 0,$$

$$\alpha_2 = 2\Re z\, \alpha_1 + \beta_1 = 2\Re z, \quad \beta_2 = -|z|^2$$

$$\Longrightarrow \qquad z^2 = 2\Re z\, z - |z|^2.$$

The sequence $\{\alpha_j\}$ can be written as a difference equation of order two with constant coefficients.

$$\alpha_{j+1} = 2\Re z\, \alpha_j - |z|^2 \alpha_{j-1}\,, \quad j = 0, 1, \ldots$$

Then for $z \notin \mathbb{R}$, the closed form of the solution for α_j reads

$$\alpha_j = \frac{\Im\{u_1^j\}}{\sqrt{|z|^2 - (\Re z)^2}},\ u_1 := \Re z + \mathbf{i}\sqrt{|z|^2 - (\Re z)^2},\ \sqrt{|z|^2 - (\Re z)^2} > 0, j \geq 0, \tag{6}$$

where u_1 is one of the two complex solutions of $u^2 - 2\Re z\, u + |z|^2 = 0$.

Remark The similar iteration as in (5) was given by Pogorui and Shapiro, 2004. They used a three term recursion whereas our recursion is a two term recursion. Thus, they differ, formally. In some cases two term recursions are more stable, than the corresponding three term recursions. For an example, see Laurie, 1999.

All powers of a quaternion

By means of (5), the polynomial p_n can be written as

$$p_n(z) = \sum_{j=0}^{n} a_j z^j = \sum_{j=0}^{n} a_j(\alpha_j z + \beta_j) = \Big(\sum_{j=0}^{n} \alpha_j a_j\Big) z + \sum_{j=0}^{n} \beta_j a_j =: A(z)z + B(z). \quad (7)$$

Theorem Let $z_0 \in \mathbb{H}$ be fixed. Then both $A(z)$ and $B(z)$ are constant for all $z \in [z_0]$. Let z_0 be a zero of p_n. Then,

$$p_n(z_0) = A(z)z_0 + B(z) = 0 \text{ for all } z \in [z_0]. \quad (8)$$

The quantities A, B in (8) can only vanish simultaneously. If $A(z_0) = 0$ and if z_0 is not real, then, z_0 generates a spherical zero of p_n. If $A(z_0) \neq 0$, then z_0 is an isolated zero.

Proof From (5) it is clear, that the coefficients $\alpha_j, \beta_j, j \geq 0$, are the same for all z with the same $\Re z, |z|$. Thus, the coefficients are the same for all $z \in [z_0]$, therefore, $A(z) = \mathrm{const},\ \mathrm{B(z)} = \mathrm{const}$ for all $z \in [z_0]$. If $A(z_0) = 0$, then necessarily $B(z_0) = 0$, and vice versa. And $p(z) = 0$ for all $z \in [z_0]$. This implies that z_0 generates a spherical zero if z_0 is not real. Recall, that $z_0 \neq 0$. Let $A(z_0) \neq 0$ and z_0 be not isolated. This case leads to a contradiction as shown in the next theorem.

Theorem Let $z_0, z_1 \in \mathbb{H}$ be two different zeros of p_n with $z_0 \in [z_1]$. Then $p_n(z) = 0$ for all $z \in [z_1]$, z_0 generates a spherical zero of p_n, and $A(z) = B(z) = 0$ for all $z \in [z_0]$.
In particular, $z_0 \notin \mathbb{R}$ is a spherical zero of p_n if and only if $A(z_0) = 0$.

Proof Since z_0, z_1 are assumed to be different and to belong to the same equivalence class, they cannot be real. From (8) it follows that

$$p_n(z_j) = A(z)z_j + B(z) = 0 \quad \text{for all} \quad z \in [z_0] = [z_1],\ j = 0, 1.$$

Taking differences, we obtain

$$p_n(z_0) - p_n(z_1) = A(z)(z_0 - z_1) = 0 \quad \text{for all} \quad z \in [z_1] = [z_0],$$

implying $A(z) = 0$. According to the preceding Theorem, the zero z_0 generates a spherical zero of p_n. If $A(z_0) \neq 0$, the zero, z_0, cannot be spherical. See also Pogorui and Shapiro, 2004.

Classification of zeros of one-sided quaternionic polynomials

Thus, we have the following classification of zeros z_0 of p_n given in (4):

- z_0 is real. By definition, z_0 is isolated.
- z_0 is not real.
  - $A(z_0) = 0 \ \Rightarrow z_0$ is spherical, all $z \in [z_0]$ are zeros of p_n
  - $A(z_0) \neq 0 \ \Rightarrow z_0$ is isolated.

Example (SIAM J. Numer. Anal. **48** (2010) Let

$$p_6(z) := z^6 + \mathbf{j}\,z^5 + \mathbf{i}z^4 - z^2 - \mathbf{j}\,z - \mathbf{i}.$$

There are the following five zeros:

1. $z_{1,2} = \pm 1$ are two real, isolated zeros;
2. $z_3 = \mathbf{i}$ is a spherical zero;
3. $z_4 := (1, -1, -1, -1)/2, \quad z_5 := (-1, 1, -1, -1)/2$ are two isolated zeros.

The computation of all zeros of p_n, including their types, can be reduced to the computation of all zeros of a real polynomial of degree $2n$.

The companion polynomial

Let p_n be a one sided quaternionic polynomial with the quaternionic coefficients $a_0, a_1, \ldots, a_n$. We define the polynomial q_{2n} of degree $2n$ with real coefficients by

$$q_{2n}(z) := \sum_{j,k=0}^{n} \overline{a_j} a_k z^{j+k} = \sum_{k=0}^{2n} b_k z^k, \quad z \in \mathbb{C}, \text{ where} \tag{9}$$

$$b_k := \sum_{j=\max(0,k-n)}^{\min(k,n)} \overline{a_j} a_{k-j} \in \mathbb{R}, \quad k = 0, 1, \ldots, 2n. \tag{10}$$

We will call q_{2n} the companion polynomial of the quaternionic polynomial p_n.
It always should be regarded as a polynomial over $\mathbb{C}$, not over **H**.
The companion polynomial q_{2n} has real coefficients, we may assume that it is always possible to find all (real and complex) zeros of q_{2n}.

How are the quaternionic zeros of p_n

related to the real or complex zeros of q_{2n}?

The idea of the companion polynomial comes from Niven (1941) or more recently from Pogorui and Shapiro (2004).

Lemma Let $p_n(z) = Az + B$, $A = A(z)$, $B = B(z)$, see (7). Then

$$q_{2n}(z) = |A|^2 z^2 + 2\Re(\overline{A}B)z + |B|^2. \tag{11}$$

Proof Let $z^j = \alpha_j z + \beta_j$. Then, we have

$$\begin{aligned} q_{2n}(z) &= \sum_{j,k=0}^{n} \overline{a_j} a_k z^{j+k} = \sum_{j=0}^{n} \overline{a_j} \left(\sum_{k=0}^{n} a_k z^k \right) z^j = \sum_{j=0}^{n} \overline{a_j}(Az + B) z^j \\ &= \sum_{j=0}^{n} \overline{a_j}(Az + B)(\alpha_j z + \beta_j) \quad [\alpha_j, \beta_j \in \mathbb{R}] \\ &= \sum_{j=0}^{n} (\alpha_j \overline{a_j}) A z^2 + \sum_{j=0}^{n} (\beta_j \overline{a_j}) A z + \sum_{j=0}^{n} (\alpha_j \overline{a_j}) B z + \sum_{j=0}^{n} (\beta_j \overline{a_j}) B \\ &= |A|^2 z^2 + 2\Re(\overline{A}B)z + |B|^2. \end{aligned}$$

Thus, the formula (11) is correct.

Theorem (real zeros) Let $z_0 \in \mathbb{R}$. Then,

$$q_{2n}(z_0) = 0 \iff p_n(z_0) = 0.$$

The set of real zeros is the same for p_n and for q_{2n}.

Proof On the real line $z \in \mathbb{R}$, we have $q_{2n}(z) = |p_n(z)|^2$.

Remark Since q_{2n} has real coefficients and $q_{2n}(z) = |p_n(z)|^2$ for $z \in \mathbb{R}$, the zeros of q_{2n} come always in pairs

$$\ldots r, r, \ldots, a + \mathbf{i}b, a - \mathbf{i}b, \ldots, \qquad r, a, b \in \mathbb{R}.$$

Theorem (spherical zeros) Let z_0 be a non real zero of q_{2n} and let $A(z_0) = 0$, far A see (7). Then, z_0 generates a spherical zero of p_n.

Proof Equation (8) implies that $B(z_0) = 0$ as well, where the quaternion B is also defined in (7). Thus, $p_n(z_0) = 0$ and z_0 generates a spherical zero of p_n.

The last case: we have to investigate non real zeros x of q_{2n} for which $A(x) \neq 0$. In general, we have $p_n(x) \neq 0$. However, we try to find a $z \in [x]$ such that $p_n(z) = 0$. If that is possible, it follows from (8) and (7) that z must necessarily have the form

$$z := -A(x)^{-1}B(x) = -\frac{\overline{A(x)}B(x)}{|A(x)|^2}. \qquad (12)$$

We have to show, that $z \in [x]$, i.e. that $\Re z = \Re x$ and $|z| = |x|$.

Lemma Let x be a non real zero of q_{2n} with $A(x) \neq 0$. Then for z in (12), we have

$$\Re z = \Re x \text{ and } |z| = |x|.$$

Let us set

$$x = (x_1, x_2, 0, 0); \quad z := (z_1, z_2, z_3, z_4); \quad \overline{A}B := (v_1, v_2, v_3, v_4). \qquad (13)$$

Theorem Let p_n be given and let q_{2n} be the corresponding companion polynomial. Assume that x is a non real, complex zero of q_{2n} with the property that $A(x) \neq 0$. Then, z in (12) is an isolated zero of p_n. Moreover, z can be written in the form

$$z = (x_1, -\frac{|x_2|}{|v|}v_2, -\frac{|x_2|}{|v|}v_3, -\frac{|x_2|}{|v|}v_4). \qquad (14)$$

Is it possible that p_n has a zero which
we do not find by checking all zeros of q_{2n}?

Theorem Let $p_n(z) = 0$ where p_n is one sided quaternionic polynomial. Then, there is an $x \in \mathbb{C}$ with $x \in [z]$ such that $q_{2n}(x) = 0$, where q_{2n} is the companion polynomial of p_n.

Conclusion

- The proposed algorithm finds all zeros of the one sided quaternionic polynomial p_n.
- The set of zeros consists of at least one and at most n elements, where the spherical zeros of the same equivalence class count as one zero.

Example

Example Let

$$p_6(z) := z^6 + \mathbf{j}z^5 + \mathbf{i}z^4 - z^2 - \mathbf{j}z - \mathbf{i}.$$

Then, the companion polynomial for p_6 is

$$q_{12}(x) = x^{12} + x^{10} - x^8 - 2x^6 - x^4 + x^2 + 1.$$

The twelve zeros of q_{12} are

$$1 \text{ (twice)}, \quad -1 \text{ (twice)}, \quad \pm\mathbf{i} \text{ (twice each)}, \quad 0.5\,(\pm 1 \pm \mathbf{i}).$$

There are two different, real zeros, $z_{1,2} = \pm 1$ which are also zeros of p_6.
There is one spherical zero, $z_3 = \mathbf{i}$, of p_6 ($-\mathbf{i}$ generates the same spherical zero).
And, finally there are two isolated zeros which have to be computed from $x = 0.5\,(\pm 1 \pm \mathbf{i})$ by formula (14). This formula yields

$$z_4 := 0.5\,(1, -1, -1, -1), \quad z_5 := 0.5\,(-1, 1, -1, -1).$$

Numerical consideration

The polynomial in the example has the property that $p_6(z) = (z^2 + \mathbf{j}z + \mathbf{i})(z^4 - 1)$. Normally, one is not able to guess the zeros. If we compute the zeros of q_{12} by MATLAB computation (results are listed in Table 1) they are not as precise as desired, though the integer coefficients of q_{12} are exact.

Table 1. Zeros of q_{12} by MATLAB computations and correct values.

1	-1.00000000000000	$+0.00000001131891\mathbf{i}$	-1
2	-1.00000000000000	$-0.00000001131891\mathbf{i}$	-1
3	-0.50000000000000	$+0.86602540378444\mathbf{i}$	$0.5(-1 + \sqrt{3}\,\mathbf{i})$
4	-0.50000000000000	$-0.86602540378444\mathbf{i}$	$0.5(-1 - \sqrt{3}\,\mathbf{i})$
5	1.00000000000000	$+0.00000001376350\mathbf{i}$	1
6	1.00000000000000	$-0.00000001376350\mathbf{i}$	1
7	0.50000000000000	$+0.86602540378444\mathbf{i}$	$0.5(1 + \sqrt{3}\,\mathbf{i})$
8	0.50000000000000	$-0.86602540378444\mathbf{i}$	$0.5(1 - \sqrt{3}\,\mathbf{i})$
9	0.00000000001566	$+1.00000000619055\mathbf{i}$	$\mathbf{i}$
10	0.00000000001566	$-1.00000000619055\mathbf{i}$	$-\mathbf{i}$
11	-0.00000000001566	$+0.99999999380945\mathbf{i}$	$\mathbf{i}$
12	-0.00000000001566	$-0.99999999380945\mathbf{i}$	$-\mathbf{i}$

Remarks

The four zeros with multiplicity one, numbered 3,4,7,8 in Table 1, are precise to machine precision, however, all other zeros, which are zeros with multiplicity 2 have errors of magnitude 10^{-8}. It is easy to improve these zeros. If z is one of the zeros with multiplicity two, an application of one step of Newton's method applied to $q'_{2n} = 0$ with starting point z is sufficient to obtain machine precision. For zeros of multiplicity four one should apply Newton's method to $q'''_{2n} = 0$, etc., possibly with two steps.

We made some hundred tests with polynomials p_n of degree $n \leq 50$ with random integer coefficients in the range $[-5, 5]$ and with real coefficients in the range $[0, 1]$. In all cases we found only (non real) isolated zeros z. The test cases showed $|p_n(z)| \approx 10^{-13}$. Real zeros and spherical zeros did not show up. If n is too large, say $n \approx 100$, then it is usually not any more possible to find all zeros of the companion polynomial by standard means (say `roots` in MATLAB) because the coefficients of the companion polynomial are too large.

Algorithm for finding zeros of one sided polynomial

$$(4') \quad p_n(z) := \sum_{j=0}^{n} a_j z^j, \quad z, a_j \in \mathbb{H}, \quad j = 0, 1, \ldots, n, \; a_n = 1\,, a_0 \neq 0, \; n \geq 1$$

1. Compute the real coefficients $b_0, b_1, \ldots, b_{2n}$ of the companion polynomial q_{2n} by formula (10). Make sure that they are real.
2. Compute all $2n$ (real and complex) zeros of q_{2n}, (in MATLAB, use the command `roots`). Denote these zeros by $z_1, z_2, \ldots, z_{2n}$ and order these zeros (if necessary) such that $z_{2j-1} = \overline{z_{2j}}$, $j = 1, 2, \ldots, n$. If a specific z_{2j_0-1} is real, then, it means that $z_{2j_0-1} = z_{2j_0}$.

3 Define an integer vector `ind` (like "indicator") of length n and set all components to zero. Define a quaternionic vector Z of length n and set all components to zero.
For `j:=1:n` do Put $z := z_{2j-1}$.

  (a) `if` z is real, $Z(j) := z$; go to the next step; `end if`
  (b) Compute $v := \overline{A(z)}B(z)$ by formula (7), with the help of formulas (5).
  (c) `if` $v = 0$, put `ind`$(j) := 1$; $Z(j) := z$; go to the next step; `end if`
  (d) `if` $v \neq 0$, let $(v_1, v_2, v_3, v_4) := v$. Compute $|w| := \sqrt{v_2^2 + v_3^3 + v_4^2}$, put

$$(14') \qquad Z(j) := \left(\Re(z), -\frac{|\Im(z)|}{|w|}v_2, -\frac{|\Im(z)|}{|w|}v_3, -\frac{|\Im(z)|}{|w|}v_4\right).$$

`end if`; `end for`

Polynomials with coefficients on the right side of the powers

Let

$$\tilde{p}_n(z) := \sum_{j=0}^{n} z^j a_j, \quad z, a_j \in \mathbb{H}, \quad j = 0, 1, 2, \ldots, n, \quad a_0\, a_n \neq = 0\,. \qquad (15)$$

be a given polynomial with coefficients on the right side of the powers.
We apply the former theory to

$$p_n(z) := \overline{\tilde{p}_n(\overline{z})} = \sum_{j=0}^{n} \overline{a}_j z^j, \quad z, a_j \in \mathbb{H}, \quad j = 0, 1, 2, \ldots, n, \quad a_0\, a_n \neq = 0. \qquad (16)$$

Lemma The two polynomials

$$\tilde{p}_n(z) := \sum_{j=0}^{n} z^j a_j \quad \text{and} \quad p_n(z) := \sum_{j=0}^{n} \overline{a}_j z^j$$

have the same real and spherical zeros.

Two-sided type quaternionic polynomials

$$p(z) := \sum_{j=0}^{n} a_j z^j b_j, \quad z,\ a_j,\ b_j \in \mathbb{H},\ a_0 b_0 \neq 0, a_n b_n \neq 0, \tag{17}$$

A general, quaternionic polynomial consists of a sum of monomials of degree j, $t_j(z) := a_{0j} \cdot z \cdot a_{1j} \cdots a_{j-1,j} \cdot z \cdot a_{jj}, \quad z, a_{0j}, a_{1j}, \ldots, a_{jj} \in \mathbb{H},\ j \geq 0.$ Since there may be several terms of the same degree we have to enumerate the terms. We do that in the form

$$t_{jk}(z) := a_{0j}^{(k)} \cdot z \cdot a_{1j}^{(k)} \cdots a_{j-1,j}^{(k)} \cdot z \cdot a_{jj}^{(k)}, \quad k = 1, 2, \ldots, k_j,\ k_j \geq 0. \tag{18}$$

The case $k_j = 0$ means that there is no monomial of degree j. A general, quaternionic polynomial of degree n takes the form

$$p(z) := \sum_{j=0}^{n} \sum_{k=1}^{k_j} t_{jk}(z). \tag{19}$$

Let $z \in \mathbb{R}$ be a real zero of p, defined in (19). Since a real z commutes with all quaternions the polynomial can be in this case written in the form

$$p(z) = \sum_{j=0}^{n} A_j z^j \text{ where } A_j := \sum_{k=1}^{k_j} a_{0j}^{(k)} a_{1j}^{(k)} \cdots a_{jj}^{(k)},\ z \in \mathbb{R}. \tag{20}$$

Example

Let $z \in \mathbb{R}$,

$$p(z) := z^2 + azbzc + dze + f. \tag{21}$$

The polynomial (20) reads in this case

$$p(z) = (1 + abc)z^2 + dez + f.$$

We choose

$$a := \mathbf{i},\ b := \mathbf{j},\ c := -\mathbf{k},\ d := \mathbf{i} + \mathbf{j},\ e := \mathbf{j} + \mathbf{k},\ f := -1 - \mathbf{i} + \mathbf{j} - \mathbf{k}.$$

Then $p(z) = 2z^2 + (-1, 1, -1, 1)z + (-1, -1, 1, -1)$.

The companion polynomial q of degree four has one as a double zero and no other real zero. Thus, the polynomial p in (21) has exactly one real zero, namely one. If in the general case the companion polynomial q has no real zero, then also the given polynomial p in (19) has no real zero. Because of these results we will concentrate to non real zeros in the sequel.

Now, we will treat the two–sided quaternionic polynomial in the form (17). To the polynomials with multiple terms of the same degree we will return later.

Types of zeros of two sided polynomials

We will again use the iteration process (5) for computing of α, β in $z^j = \alpha z + \beta$ with real α, β, and also the closed form solution obtained by using the theory of difference equations for α_j in the case $z \notin \mathbb{R}$, namely the formula (6).

By means of (5) the polynomial p can be written as

$$p(z) := \sum_{j=0}^{n} a_j z^j b_j = \sum_{j=0}^{n} a_j(\alpha_j z + \beta_j) b_j \tag{22}$$

$$= \sum_{j=0}^{n} \alpha_j a_j z b_j + \sum_{j=0}^{n} \beta_j a_j b_j = C(z) + B(z), \text{ where} \tag{23}$$

$$C(z) := \sum_{j=0}^{n} \alpha_j a_j z b_j, \quad B(z) := \sum_{j=0}^{n} \beta_j a_j b_j. \tag{24}$$

Lemma Let C be defined as in (24). Then, $C : \mathbb{R}^4 \to \mathbb{R}^4$ is a linear mapping over $\mathbb{R}$. Let z_0 be non real. Then, $B(z)$, defined in (24), is constant for $z \in [z_0]$. If $p(z) = 0$ for some $z \in \mathbb{H}$, then $C(z) = B(z) = 0$ or $C(z) \neq 0$ and $B(z) \neq 0$.

Isomorphic matrix representation for quaternions

We introduce two mappings $\omega_1, \omega_2 : \mathbb{H} \to \mathbb{R}^{4\times 4}$ by

$$\omega_1(a) := \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ a_2 & a_1 & -a_4 & a_3 \\ a_3 & a_4 & a_1 & -a_2 \\ a_4 & -a_3 & a_2 & a_1 \end{pmatrix} \in \mathbb{R}^{4\times 4}, \tag{25}$$

$$\omega_2(a) := \begin{pmatrix} a_1 & -a_2 & -a_3 & -a_4 \\ a_2 & a_1 & a_4 & -a_3 \\ a_3 & -a_4 & a_1 & a_2 \\ a_4 & a_3 & -a_2 & a_1 \end{pmatrix} \in \mathbb{R}^{4\times 4}. \tag{26}$$

The first mapping ω_1 represents the isomorphic image of a quaternion $a = (a_1, a_2, a_3, a_4)$ in the matrix space $\mathbb{R}^{4\times 4}$. Thus, we have

$$\omega_1(ab) = \omega_1(a)\omega_1(b).$$

The second mapping ω_2 (Aramanovitch, 1995) has the remarkable property that it reverses the multiplication order

$$\omega_2(ab) = \omega_2(b)\omega_2(a).$$

The two matrices $\omega_1(a), \omega_2(b)$ coincide if and only if $a = b \in \mathbb{R}$.

Remark From the definition (25), (26) it follows that

$$\omega_1(a)^{\mathrm{T}} = \omega_1(\bar{a}), \qquad \omega_2(b)^{\mathrm{T}} = \omega_1(\bar{b}). \tag{27}$$

Both matrices are orthogonal in the sense

$$\omega_1(a)\omega_1(a)^{\mathrm{T}} = \omega_1(a)\omega_1(\bar{a}) = |a|^2\,\mathbf{I}, \quad \omega_2(b)\omega_2(b)^{\mathrm{T}} = |b|^2\,\mathbf{I}.$$

Let $a := (a_1, a_2, a_3, a_4) \in \mathbb{H}$. We introduce a simple, but very useful column operator $\mathrm{col} : \mathbb{H} \to \mathbb{R}^4$ by

$$\mathrm{col}(a) := \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix},$$ a quaternion as a matrix with one column and four rows.

Lemma The column operator is linear over $\mathbb{R}$, i. e.

$$\mathrm{col}(\alpha a + \beta b) = \alpha\mathrm{col}(a) + \beta\mathrm{col}(b), \quad a, b \in \mathbb{H}, \alpha, \beta \in \mathbb{R}.$$

Lemma For arbitrary quaternions a, b, c we have

$$\mathrm{col}(ab) = \omega_1(a)\mathrm{col}(b) = \omega_2(b)\mathrm{col}(a), \tag{28}$$

$$\mathrm{col}(abc) = \omega_1(a)\omega_2(c)\mathrm{col}(b). \tag{29}$$

Let us put $\omega_3(a, b) := \omega_1(a)\omega_2(b) \in \mathbb{R}^{4\times 4}, \quad a, b \in \mathbb{H}.$

Lemma The matrix $\omega_3(a,b)$ is normal and orthogonal in the sense

$$\omega_3(a,b)^{\mathrm{T}}\omega_3(a,b) = \omega_3(a,b)\omega_3(a,b)^{\mathrm{T}} = |a|^2|b|^2\,\mathbf{I}.$$

Thus, all eigenvalues of $\omega_3(a,b)$ have the same absolute value $|a||b|$.

Theorem Let $p(z) := C(z) + B(z)$ be defined as in (22) to (24). Then,

$$\mathrm{col}(p(z)) = \left(\sum_{j=0}^{n} \alpha_j \omega_3(a_j, b_j)\right) \mathrm{col}(z) + \sum_{j=0}^{n} \beta_j \mathrm{col}(a_j b_j) \tag{30}$$

$$=: \mathbf{A}(z)\mathrm{col}(z) + \mathrm{col}(B(z)), \text{ where} \tag{31}$$

$$\mathbf{A}(z) := \left(\sum_{j=0}^{n} \alpha_j \omega_3(a_j, b_j)\right) \in \mathbb{R}^{4\times 4}, \ \mathrm{col}(B(z)) := \sum_{j=0}^{n} \beta_j \mathrm{col}(a_j b_j). \tag{32}$$

Lemma Let z_0 be non real. Then, the matrix $\mathbf{A}(z)$, defined in (32), is constant for $z \in [z_0]$.

Instead of considering the equation $p(z) = 0$ we consider the equivalent equation

$$P(z) := \mathrm{col}(p(z)) = \mathbf{A}(z)\mathrm{col}(z) + \mathrm{col}(B(z)) = \mathrm{col}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 0. \quad (33)$$

Theorem Let z be a non real zero of p such that equation (33) is valid. Then, this equation remains valid if in $\mathbf{A}(z)$, $B(z)$ the zero z is replaced with the complex representative z_0 of $[z]$.

Corollary In order to find the non real zeros $z \in \mathbb{H}$ of p, defined in (17), it is sufficient to find the complex representatives z_0 of $[z]$.

The matrix $\mathbf{A}(z)$, occurring in (33) may be singular or non singular:

Theorem Let z_1, z_2 be two different but equivalent zeros of a polynomial p defined in (17). Then, $\mathbf{A} := \mathbf{A}(z_1) = \mathbf{A}(z_2)$, and $\mathbf{A}$ is singular, where $\mathbf{A}(z)$ is defined in (32).

Proof Let $p(z_j) = 0$ for $j = 1, 2$. Then

$$\mathrm{col}(p(z_j)) = B(z_j) + \mathbf{A}(z_j)\mathrm{col}(z_j) = 0\,.$$

We put $B := B(z_1) = B(z_2)$ and $\mathbf{A} := \mathbf{A}(z_1) = \mathbf{A}(z_2)$. Taking differences, we obtain

$$\mathrm{col}(p(z_1)) - \mathrm{col}(p(z_2)) = \mathbf{A}\mathrm{col}(z_1 - z_2) = 0\,.$$

Since $z_1 - z_2 \neq 0$, the matrix $\mathbf{A}$ must be singular.

Classification of the zeros of two–sided quaternionic polynomials

Definition Let z be a zero of p, defined in (17), and let $z_0 \in [z]$ be the complex representative of $[z]$. We classify the zeros z of p with respect to the rank of $\mathbf{A}(z_0)$.

- The zero z will be called zero of type k if $\operatorname{rank}(\mathbf{A}(z_0)) = 4 - k, 0 \leq k \leq 4$.
- A zero of type 4 $(\operatorname{rank}(\mathbf{A}(z_0)) = 0)$ will be called spherical zero. It has the property that all $z \in [z_0]$ are zeros.
- A zero of type 0 will be called isolated zero. In this case

  $$z = -(\mathbf{A}(z_0))^{-1}\operatorname{col}(B(z_0))$$

  is the only zero in $[z_0]$.
- We will also call a real zero an isolated zero.

Numerical considerations

The equations (30) to (33) read

(33) $$P(z) := \mathrm{col}(p(z)) = \mathbf{A}(z)\mathrm{col}(z) + \mathrm{col}(B(z)) = 0.$$

A standard technique for solving such a system is Newton's method. In short, this technique results in solving the following linear equation for s, repeatedly:

$$P(z) + P'(z)s = 0; \quad z := z + s, \tag{34}$$

where in the beginning one needs an initial guess z.
In order to compute the (4×4) Jacobi matrix P' we use numerical differentiation.
Let e_k, $k = 1, 2, 3, 4$ be one of the four standard unit vectors in $\mathbb{R}^4$, $z := (z_1, z_2, z_3, z_4)$. Then,

$$\frac{\partial P}{\partial z_k}(z) \approx \frac{P(z + he_k) - P(z)}{h}, \; k = 1, 2, 3, 4, \quad h \approx 10^{-7}, \tag{35}$$

$$P'(z) := \left(\frac{\partial P}{\partial z_1}(z), \frac{\partial P}{\partial z_2}(z), \frac{\partial P}{\partial z_3}(z), \frac{\partial P}{\partial z_4}(z)\right). \tag{36}$$

The choice $h \approx 10^{-7}$ is the standard choice for computers with machine precision of $\approx 10^{-15}$. This choice implies a good balance between the round off and truncation errors.

The number of zeros of quaternionsc polynomials

Since the polynomial $p(z) := z^2 + 1$ has already infinitely many zeros in $\mathbb{H}$, it makes no sense to count the individual zeros.

Definition Let p be any quaternionic polynomial of degree $n \geq 2$. By $\#Z(p)$ we understand the number of equivalence classes in $\mathbb{H}$ which contain zeros of p. We call this number, essential number of zeros of p.

By this definition, $p(z) := z^2 + 1$ has one essential zero, since $\mathbf{i}$ and $-\mathbf{i}$ are located in the same equivalence class.

All polynomials with real coefficients and degree n as well as all quaternionic, one–sided polynomials of degree n have at most n essential zeros

Theorem Let p be a quaternionic, two–sided polynomial of degree n. Then, $\#Z(p)$, the essential number of zeros of p, is, in general, not bounded by n.

Example Let $p(z) := a_3 z^3 b_3 + a_2 z^2 b_2 + a_1 z b_1 + c_0$, where

$$\begin{array}{lll} a_3 := (1,1,0,0), & b_3 := (-1,-1,-1,0), & c_0 := (2,0,0,0). \\ a_2 := (-1,0,1,1), & b_2 := (0,-1,0,1), & \\ a_1 := (0,-1,1,1), & b_1 := (1,0,0,1), & \end{array}$$

The polynomial p is of degree three and the essential number of zeros of p is five.

Conjecture Let p be a quaternionic two–sided polynomial of degree n of the form (17). Then, the essential number of zeros of p will not exceed $2n$:

$$\#Z(p) \leq 2n\,.$$

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