LOW-RANK TENSOR DECOMPOSITIONS FOR QUATERNION MULTIWAY ARRAYS

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ABSTRACT

Quaternion multiway arrays appear naturally as compact representations of 3D or 4D multidimensional signals. However, the non-commutativity of quaternion multiplication prevents a straightforward extension of standard tensor algebra to analyze and process quaternion multiway arrays. After reviewing the theoretical difficulties related to quaternion tensor algebra, we propose the first construction of quaternion tensors as representation of dedicated quaternion multilinear forms. This theoretical construction ensures that usual tensor algebraic properties, such as mode products properties are preserved. This novel framework enables us to generalize Tucker and canonical polyadic tensor decompositions to the quaternion case. For the latter, we carefully design a full quaternion ALS-type algorithm. Its relevance is validated numerically.

1. INTRODUCTION

Quaternions generalize complex numbers in four dimensions. The popularity of quaternions in signal and image processing stems from their ability to represent 3D and 4D vectors as single quaternion scalars. This enables compact algebraic representations together with many geometric insights such as 3D rotations. Multiway arrays of quaternions appear whenever 3D or 4D vector data is acquired with respect to one or more diversities (time, space, wavelength, etc.). Examples include RGB color imaging [1–4], polarized source separation [5], vector array processing [6, 7], wind and temperature forecasting [8], to cite only a few. So far, most of the research has focused on developing methodologies for dealing with quaternion vectors and matrices, which does not permit a proper account for multiple (> 2) diversities. Just like in the real and complex case, there is the need to develop a mathematically grounded framework for quaternion multiway arrays, namely a meaningful *quaternion tensor algebra*. The lack of such framework can be explained by the noncommutativity of the quaternion product, which prevents a direct extension of classical real and complex tensor definitions. A few attempts at defining tensor-like tools for quaternion multiway arrays have been made recently [9–13]. However, a proper definition of quaternion tensors based on multilinear arguments remains to be established to unlock the development of meaningful tensor algebra tools in the quaternion case. After explaining the difficulties inherent to the construction of such a mathematical object, we propose a definition of quaternion tensors preserving usual properties of tensor calculus. We revisit the main tensor decompositions, Tucker and the Canonical Polyadic Decomposition (CPD), for this new object. Finally, we introduce a full quaternion domain ALS-like algorithm for the estimation of the CPD model, whose relevance is demonstrated by several numerical simulations.

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2. PRELIMINARIES

Quaternions. They define a four-dimensional noncommutative division algebra $\mathbb{H}$ over the real numbers $\mathbb{R}$ with canonical basis $\{1, \boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}\}$. Here, $\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k}$ are imaginary units satisfying $\boldsymbol{i}^2 = \boldsymbol{j}^2 = \boldsymbol{k}^2 = \boldsymbol{ijk} = -1$, $\boldsymbol{ij} = -\boldsymbol{ji}$ and $\boldsymbol{ij} = \boldsymbol{k}$. Noncommutativity of quaternion multiplication implies that for any $p, q \in \mathbb{H}$, one has $pq \neq qp$ in general. A quaternion $q \in \mathbb{H}$ can be written as $q = q_a + \boldsymbol{i}q_b + \boldsymbol{j}q_c + \boldsymbol{k}q_d$, where $q_a, q_b, q_c, q_d \in \mathbb{R}$ are its four components. The real part of q is $\operatorname{Re} q = q_a$ and its imaginary part is $\operatorname{Im} q = \boldsymbol{i}q_b + \boldsymbol{j}q_c + \boldsymbol{k}q_d$. The conjugate of q is defined as $q^* = \operatorname{Re} q - \operatorname{Im} q$ and its modulus $|\mathbf{q}| = \sqrt{qq^*} = \sqrt{q^*q} = \sqrt{q_a^2 + q_b^2 + q_c^2 + q_d^2}$. For any $p, q \in \mathbb{H}$, one has $(pq)^* = q^*p^*$.

Quaternion linear algebra. Similarly to the real and complex cases, quaternions vectors and matrices can be defined as 1D and 2D quaternions arrays, respectively. A quaternion vector $\boldsymbol{q} \in \mathbb{H}^N$ is specified by its entries $(\boldsymbol{q})_i = q_i \in \mathbb{H}$ and a quaternion matrix $\boldsymbol{A} \in \mathbb{H}^{M\times N}$ by its elements $(\boldsymbol{A})_{ij} = a_{ij} \in \mathbb{H}$. The transpose of $\boldsymbol{A}$ is denoted by $\boldsymbol{A}^\mathsf{T}$ and its conjugate-transpose (or Hermitian) by $\boldsymbol{A}^\mathsf{H} \triangleq (\boldsymbol{A}^*)^\mathsf{T} = (\boldsymbol{A}^\mathsf{T})^*$. Importantly, noncommutativity of quaternion multiplication imposes to consider two separate definitions for the quaternion matrix product. Given $\boldsymbol{A} \in \mathbb{H}^{M\times N}, \boldsymbol{B} \in \mathbb{H}^{N\times P}$, one distinguishes between *left* and *right* quaternion matrix products:

$$(\boldsymbol{A} \cdot_L \boldsymbol{B})_{ij} \triangleq \sum_{k=1}^{N} a_{ik}b_{kj} \quad \text{and} \quad (\boldsymbol{A} \cdot_R \boldsymbol{B})_{ij} \triangleq \sum_{k=1}^{N} b_{kj}a_{ik}\,.$$

Note that $\boldsymbol{A} \cdot_L \boldsymbol{B} \neq \boldsymbol{A} \cdot_R \boldsymbol{B}$ in general. These two products satisfy several different algebraic properties [14] such as:

- transposition : $(\boldsymbol{A} \cdot_{L,R} \boldsymbol{B})^{\mathsf{T}} = \boldsymbol{B}^{\mathsf{T}} \cdot_{R,L} \boldsymbol{A}^{\mathsf{T}}$;
- conjugation : $(\boldsymbol{A} \cdot_{L,R} \boldsymbol{B})^{*} = \boldsymbol{A}^{*} \cdot_{R,L} \boldsymbol{B}^{*}$;
- conjugate-transposition : $(\boldsymbol{A} \cdot_{L,R} \boldsymbol{B})^{\mathsf{H}} = \boldsymbol{B}^{\mathsf{H}} \cdot_{L,R} \boldsymbol{A}^{\mathsf{H}}$.

For more details on quaternion linear algebra, we refer the reader to [15, 16] and the references therein.

Quaternion vector spaces. Extending the notion of vector space to quaternions is relatively straightforward [17]. Nonetheless, noncommutativity of quaternion multiplication imposes once again the distinction between left and right vector spaces, depending from which side the scalar multiplication is performed. Subscripts $_L$ and $_R$ indicate the nature of the vector space considered. For instance, $\mathbb{H}_L^M$ is a left quaternion vector space of dimension M: for every $\boldsymbol{q} \in \mathbb{H}_L^M$ and every $\lambda \in \mathbb{H}$, left linearity reads $\lambda \boldsymbol{q} \in \mathbb{H}_L^M$. The approach holds for right quaternion vector spaces such as $\mathbb{H}_R^M$, where $\forall \boldsymbol{q} \in \mathbb{H}_R^M, \forall \lambda \in \mathbb{H}, \boldsymbol{q}\lambda \in \mathbb{H}_R^M$.

3. TENSORS ON $\mathbb{H}$: DEFINITIONS, PROPERTIES

3.1. Quaternion multilinearity: a wild goose chase?

Consider D quaternion vector spaces $\mathcal{S}_d$, $1 \leq d \leq D$. For now, we do not specify left or right linearity. Let $f : \mathcal{S}_1 \times \mathcal{S}_2 \times \ldots \times \mathcal{S}_D \to \mathbb{H}$ be a quaternion-valued function of D quaternion vector variables. If we require f to belong to a class of multilinear functions (f be linear in each one of its D arguments), then several important issues must be faced. The particular case $D = 3$ is sufficient to illustrate our purpose. Let $f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$ be left-linear in each argument, that is $\forall \alpha, \beta \in \mathbb{H}, \forall \boldsymbol{x}_d, \boldsymbol{y}_d \in \mathcal{S}_d$ $(d = 1, 2, 3)$:

$$f(\alpha \boldsymbol{x}_1 + \beta \boldsymbol{y}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) = \alpha f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) + \beta f(\boldsymbol{y}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) \quad (1)$$

$$f(\boldsymbol{x}_1, \alpha \boldsymbol{x}_2 + \beta \boldsymbol{y}_2, \boldsymbol{x}_3) = \alpha f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) + \beta f(\boldsymbol{x}_1, \boldsymbol{y}_2, \boldsymbol{x}_3) \quad (2)$$

$$f(\boldsymbol{x}_1, \boldsymbol{x}_2, \alpha \boldsymbol{x}_3 + \beta \boldsymbol{y}_3) = \alpha f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) + \beta f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{y}_3) \quad (3)$$

Computing $f(\alpha \boldsymbol{x}_1, \beta \boldsymbol{x}_2, \boldsymbol{x}_3)$ for $\alpha, \beta \in \mathbb{H}$ is then troublesome. Indeed changing the order in which linearity properties (1) – (3) are applied yields different results. Starting with (1) and then (2) gives $f(\alpha \boldsymbol{x}_1, \beta \boldsymbol{x}_2, \boldsymbol{x}_3) = \alpha\beta f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$, whereas applying the reversed order yields $f(\alpha \boldsymbol{x}_1, \beta \boldsymbol{x}_2, \boldsymbol{x}_3) = \beta\alpha f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$. Since multiplication in $\mathbb{H}$ is noncommutative, $\alpha\beta \neq \beta\alpha$ and thus $\beta\alpha f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3) \neq \alpha\beta f(\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3)$. Similar contradictions are observed for any other choice of variables or change of linearity properties of f and $\mathcal{S}_d$ (all right-linear, mixed between left and right-linear). Therefore, in general, there is *no such thing as quaternion multilinearity*. This might explain the scarcity of theoretical results on quaternion-valued tensors in the literature.

3.2. A general class of quaternion linear forms

To workaround this intrinsic quaternion multilinearity issue, we propose a general class of quaternion-valued (multi-)linear forms that satisfies several important elementary properties while preserving the nice algebraic calculus of quaternions. The definition of this class is the cornerstone of the proposed quaternion tensors framework introduced in the next section. In order to extend relevant multilinearity-like properties to the quaternion linear form f, it is necessary to restrict the nature of the different vectors spaces $\mathcal{S}_d$ defining the domain of f. More precisely, let us suppose that:

- $\mathcal{S}_1 = \mathbb{H}_L^{N_1}$ is a *left* quaternion vector space;
- $\mathcal{S}_D = \mathbb{H}_R^{N_D}$ is a *right* quaternion vector space;
- $\mathcal{S}_2 = \mathbb{R}^{N_2}, \ldots, \mathcal{S}_{D-1} = \mathbb{R}^{N_{D-1}}$ are *real* vector spaces.

This setting defines a class of quaternion-valued linear forms $f : \mathbb{H}_L^{N_1} \times \mathbb{R}^{N_2} \times \ldots \times \mathbb{R}^{N_{D-1}} \times \mathbb{H}_R^{N_D} \to \mathbb{H}$ that satisfies multilinearity properties specific to quaternion algebra:

- left quaternion linearity for $d = 1$:

$$\begin{gathered} \forall \alpha, \beta \in \mathbb{H}, \boldsymbol{x}_1, \boldsymbol{y}_1 \in \mathbb{H}_L^{N_1} \\ f(\alpha \boldsymbol{x}_1 + \beta \boldsymbol{y}_1, \ldots) = \alpha f(\boldsymbol{x}_1, \ldots) + \beta f(\boldsymbol{y}_1, \ldots); \end{gathered} \quad (4)$$

- right quaternion linearity for $d = D$:

$$\begin{gathered} \forall \alpha, \beta \in \mathbb{H}, \forall \boldsymbol{x}_D, \boldsymbol{y}_D \in \mathbb{H}_R^{N_D} \\ f(\ldots, \boldsymbol{x}_D \alpha + \boldsymbol{y}_D \beta) = f(\ldots, \boldsymbol{x}_D)\alpha + f(\ldots, \boldsymbol{y}_D)\beta; \end{gathered} \quad (5)$$

- real linearity for $2 \leq d \leq D - 1$:

$$\begin{aligned} &\forall \alpha, \beta \in \mathbb{R}, \forall \boldsymbol{x}_d, \boldsymbol{y}_d \in \mathbb{R}_R^{N_d} \\ &f(\ldots, \alpha \boldsymbol{x}_d + \beta \boldsymbol{y}_d, \ldots) = f(\ldots, \boldsymbol{x}_d \alpha + \boldsymbol{y}_d \beta, \ldots) \\ &= \alpha f(\ldots, \boldsymbol{x}_d, \ldots) + \beta f(\ldots, \boldsymbol{y}_d, \ldots) \\ &= f(\ldots, \boldsymbol{x}_d, \ldots)\alpha + f(\ldots, \boldsymbol{y}_d, \ldots)\beta. \end{aligned} \quad (6)$$

We call a function f satisfying (4)–(6) $\mathbb{HR}$-multilinear, since it involves a mix between real and quaternion linearity properties. It is worth noting that, if f is $\mathbb{HR}$-multilinear, by definition it is also $\mathbb{R}$-multilinear.

Remark. The ordering of left and right quaternion vector spaces together with that of the real vector spaces is completely arbitrary and can be permuted if necessary. Our convention here permits to simplify the presentation.

3.3. Quaternion tensors as quaternion linear forms

The core of the proposed approach lies in associating a quaternion tensor $\boldsymbol{\mathcal{T}}$ with a quaternion $\mathbb{HR}$-multilinear form f, as defined in Section 3.2. This approach follows a standard way to define tensors as coefficients in a given Cartesian product basis of a certain multilinear form [18]. Let $N_d = \dim \mathcal{S}_d$ and $\{\mathbf{e}_{i_d}^{(d)}\}_{i_d=1:N_d}$ be a basis of vector space $\mathcal{S}_d$. We then define

$$\mathcal{T}_{i_1 i_2 \ldots i_D} \triangleq f\left(\mathbf{e}_{i_1}^{(1)}, \mathbf{e}_{i_2}^{(2)}, \ldots, \mathbf{e}_{i_D}^{(D)}\right) \quad (7)$$

i.e. $\boldsymbol{\mathcal{T}} \in \mathbb{H}^{N_1 \times N_2 \times \ldots \times N_D}$ represents the multidimensional quaternion-valued array of coefficients of f in the Cartesian product basis $\{\mathbf{e}_{i_1}^{(1)}\}_{i_1=1:N_1} \times \ldots \times \{\mathbf{e}_{i_D}^{(D)}\}_{i_D=1:N_D}$.

3.4. n-mode product properties

The definition of a quaternion tensor (7) relies on a particular choice of the underlying vector spaces. This choice makes it possible to extend classical tensor operations to the quaternion case, while preserving essential tensor algebra properties. The n-mode product is one of these operations. Since the considered vector spaces have different linearity properties, we distinguish once again between 1-mode product, D-mode product and d-mode products ($2 \leq d \leq D-1$):

- 1-mode product defined as the left quaternion matrix product by $\boldsymbol{U} \in \mathbb{H}^{J \times N_1}$:

$$\left(\boldsymbol{\mathcal{T}} \times_1^L \boldsymbol{U}\right)_{j i_2 \ldots i_D} \triangleq \sum_{i_1=1}^{N_1} u_{j i_1} T_{i_1 i_2 \ldots i_D}. \quad (8)$$

- D-mode product defined as the right quaternion matrix product by $\boldsymbol{U} \in \mathbb{H}^{J \times N_D}$:

$$\left(\boldsymbol{\mathcal{T}} \times_D^R \boldsymbol{U}\right)_{i_1 \ldots i_{D_1} j} \triangleq \sum_{i_D=1}^{N_D} T_{i_1 i_2 \ldots i_D} u_{j i_D}. \quad (9)$$

- d-mode product defined as the real matrix product by $\boldsymbol{U} \in \mathbb{R}^{J \times N_d}$:

$$\left(\boldsymbol{\mathcal{T}} \times_d \boldsymbol{U}\right)_{i_1 \ldots j \ldots i_D} \triangleq \sum_{i_d=1}^{N_d} T_{i_1 \ldots i_d \ldots i_D} u_{j i_d}. \quad (10)$$

Note that the position of $u_{j i_d}$ is arbitrary in the last equation since it is real-valued. We use subscripts $_L$ or $_R$ to indicate the type of quaternion matrix multiplication involved. Another benefit of the definition of a quaternion tensor (7) is that it permits to preserve the classical properties of successive n-mode products [19]: (i) commutativity between distinct modes and (ii) matrix composition between identical modes. Other choices of (multilinearity) properties of f do not allow for preserving such nice, yet also fundamental, properties.

Proposition 1 (Commutativity)**.** *Let $\boldsymbol{\mathcal{T}} \in \mathbb{H}^{N_1 \times N_2 \times \ldots \times N_D}$, $\boldsymbol{U}_1 \in \mathbb{H}^{J_1 \times N_1}, \boldsymbol{U}_D \in \mathbb{H}^{J_D \times N_D}$ and $\boldsymbol{U}_d \in \mathbb{R}^{J_d \times N_d}$. The following properties are satisfied:*

$$\boldsymbol{\mathcal{T}} \times_1^L \boldsymbol{U}_1 \times_D^R \boldsymbol{U}_D = \boldsymbol{\mathcal{T}} \times_D^R \boldsymbol{U}_D \times_1^L \boldsymbol{U}_1, \quad (11)$$

$$\boldsymbol{\mathcal{T}} \times_1^L \boldsymbol{U}_1 \times_d \boldsymbol{U}_d = \boldsymbol{\mathcal{T}} \times_d \boldsymbol{U}_d \times_1^L \boldsymbol{U}_1, \quad (12)$$

$$\boldsymbol{\mathcal{T}} \times_d \boldsymbol{U}_d \times_D^R \boldsymbol{U}_D = \boldsymbol{\mathcal{T}} \times_D^R \boldsymbol{U}_D \times_d \boldsymbol{U}_d. \quad (13)$$

Proposition 2 (Composition)**.** *Let $\boldsymbol{\mathcal{T}} \in \mathbb{H}^{N_1 \times N_2 \times \ldots \times N_D}$, $\boldsymbol{U}, \boldsymbol{V}$ matrices with entries in appropriate sets ($\mathbb{H}$ or $\mathbb{R}$) and of adequate dimensions. The following properties are satisfied:*

$$\boldsymbol{\mathcal{T}} \times_1^L \boldsymbol{U} \times_1^L \boldsymbol{V} = \boldsymbol{\mathcal{T}} \times_1^L (\boldsymbol{V} \cdot_L \boldsymbol{U}), \quad (14)$$

$$\boldsymbol{\mathcal{T}} \times_D^R \boldsymbol{U} \times_D^R \boldsymbol{V} = \boldsymbol{\mathcal{T}} \times_D^R (\boldsymbol{V} \cdot_R \boldsymbol{U}), \quad (15)$$

$$\boldsymbol{\mathcal{T}} \times_d \boldsymbol{U} \times_d \boldsymbol{V} = \boldsymbol{\mathcal{T}} \times_d (\boldsymbol{V}\boldsymbol{U}). \quad (16)$$

Proofs of Prop. 1 and 2 are found by direct calculations.

4. QUATERNION TENSOR DECOMPOSITIONS

Low-rank quaternion tensor decompositions of a given tensor $\boldsymbol{\mathcal{T}}$ can now be easily formulated from successive n-modes products applied to a (core) tensor $\boldsymbol{\mathcal{S}}$ of smaller dimensions. We introduce below the Tucker and Canonical Polyadic Decompositions (Q-CPD) for quaternions tensors. For simplicity, we restrict ourselves in this section to quaternions tensors of order three – extension to higher orders is straightforward.

4.1. Quaternion Tucker decomposition

Consider a quaternion core tensor $\boldsymbol{\mathcal{S}} \in \mathbb{H}^{F_1 \times F_2 \times F_2}$ and 3 factor matrices $\boldsymbol{A} \in \mathbb{H}^{N_1 \times F_1}, \boldsymbol{B} \in \mathbb{R}^{N_2 \times F_2}, \boldsymbol{C} \in \mathbb{H}^{N_3 \times F_3}$. The Tucker decomposition of $\boldsymbol{\mathcal{T}} \in \mathbb{H}^{N_1 \times N_2 \times N_3}$ is given by:

$$\boldsymbol{\mathcal{T}} = \boldsymbol{\mathcal{S}} \times_1^L \boldsymbol{A} \times_2 \boldsymbol{B} \times_3^R \boldsymbol{C} \triangleq [\![\boldsymbol{\mathcal{S}}; \boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!]. \quad (17)$$

Each element $\mathcal{T}_{i_1 i_2 i_3}$ of $\boldsymbol{\mathcal{T}}$ reads explicitly

$$\mathcal{T}_{i_1 i_2 i_3} = \sum_{j_1=1}^{F_1} \sum_{j_2=1}^{F_2} \sum_{j_3=1}^{F_3} a_{i_1 j_1} \mathcal{S}_{j_1 j_2 j_3} b_{i_2 j_2} c_{i_3 j_3}. \quad (18)$$

Recall that, unlike the real/complex cases, quantities in (18) do not commute with one another, excepted for $b_{i_2 j_2} \in \mathbb{R}$.

4.2. Quaternion CPD

The Q-CPD can easily be deduced from the quaternion Tucker decomposition by considering a diagonal core tensor $\boldsymbol{\mathcal{S}} \in \mathbb{H}^{F \times F \times F}$ with $F = F_1 = F_2 = F_3$. The Q-CPD is written as $\boldsymbol{\mathcal{T}} = [\![\boldsymbol{\lambda}; \boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!]$, with $\boldsymbol{\lambda} \in \mathbb{H}^F$ corresponding to the diagonal of $\boldsymbol{\mathcal{S}}$. Every element $\mathcal{T}_{i_1 i_2 i_3}$ of $\boldsymbol{\mathcal{T}}$ reads:

$$\mathcal{T}_{i_1 i_2 i_3} = \sum_{f=1}^{F} a_{i_1 f} \lambda_f b_{i_2 f} c_{i_3 f}, \quad (19)$$

where $\lambda_f \in \mathbb{H}$ is interpreted as a quaternion-valued scaling factor for the fth rank-1 term of the Q-CPD.

Ambiguities. Without any loss of generality, assume that $\boldsymbol{\mathcal{S}}$ is the identity tensor such that the Q-CPD can be expressed as $\boldsymbol{\mathcal{T}} = [\![\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!]$. Then, (19) shows that even if the Q-CPD is unique, it suffers from several trivial ambiguities. The first one is classical, order ambiguity, and is obtained by joint permutation of columns of the factor matrices $\boldsymbol{\mathcal{T}} = [\![\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!] = [\![\boldsymbol{A}\boldsymbol{\Pi}, \boldsymbol{B}\boldsymbol{\Pi}, \boldsymbol{C}\boldsymbol{\Pi}]\!]$, with $\boldsymbol{\Pi} \in \mathbb{R}^{F \times F}$ a permutation matrix. In contrast, the scaling ambiguity differs from the standard real and complex cases, i.e. $\boldsymbol{\mathcal{T}} = [\![\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!] = [\![\boldsymbol{A} \cdot_L \boldsymbol{\Gamma}_1, \boldsymbol{B}\boldsymbol{\Gamma}_2, \boldsymbol{C} \cdot_R \boldsymbol{\Gamma}_3]\!]$, with $\boldsymbol{\Gamma}_1, \boldsymbol{\Gamma}_3 \in \mathbb{H}^{F \times F}$, and $\boldsymbol{\Gamma}_2 \in \mathbb{R}^{F \times F}$ diagonal matrices such that $(\boldsymbol{\Gamma}_1 \cdot_L \boldsymbol{\Gamma}_3)\boldsymbol{\Gamma}_2 = \boldsymbol{I}_F$, with $\boldsymbol{I}_F$ the $(F \times F)$ identity matrix. Provided that quaternion-valued scalings are computed with special care due to noncommutativity, practical handling of Q-CPD ambiguities follows closely that of the standard real and complex tensor case.

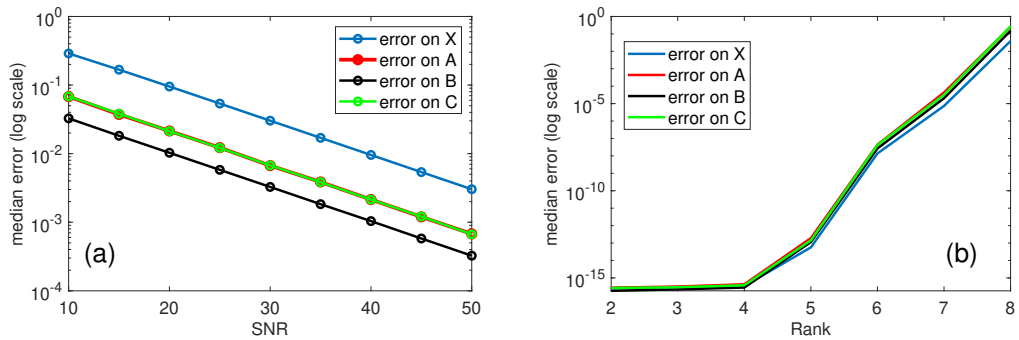

Fig. 1: Simulation results. (a) Median errors with respect to the SNR; (b) Median errors with respect to the rank (no noise)

Mode unfoldings. A key benefit of the proposed representation of quaternion tensors (7) is that one can easily write tensor mode unfoldings models for Q-CPD (19), using Khatri-Rao products as for real/complex tensors. Once again, matrix operations such as Kronecker or Khatri-Rao products must distinguish between left and right products. The three mode unfoldings of the quaternion CPD model (19) are given by

$$\boldsymbol{T}_{(1)} = \boldsymbol{A} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{B})^{\mathsf{T}}, \tag{20}$$

$$\boldsymbol{T}_{(2)} = \boldsymbol{B} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{A})^{\mathsf{T}}, \tag{21}$$

$$\boldsymbol{T}_{(3)} = \boldsymbol{C} \cdot_R (\boldsymbol{B} \odot_R \boldsymbol{A})^{\mathsf{T}}. \tag{22}$$

where $\odot_R$ denotes the right-sided Khatri-Rao product [14].

5. Q-CPD ALGORITHM

5.1. Quaternion matrix least squares

The design of a quaternion-domain CPD alternating least squares (ALS) algorithm involves solving two different kind of quaternion matrix least squares subproblems, depending on the nature (left/right) of quaternion matrix multiplication:

$$\hat{\boldsymbol{X}}_L = \underset{\boldsymbol{X}}{\operatorname{argmin}} \|\boldsymbol{M} - \boldsymbol{X} \cdot_L \boldsymbol{N}\|_{\mathsf{F}}^2, \tag{23}$$

$$\hat{\boldsymbol{X}}_R = \underset{\boldsymbol{X}}{\operatorname{argmin}} \|\boldsymbol{M} - \boldsymbol{X} \cdot_R \boldsymbol{N}\|_{\mathsf{F}}^2, \tag{24}$$

where $\|\cdot\|_{\mathsf{F}}$ denotes the Frobenius norm of a matrix. The solution to (23) is known from [20] and relies on the theory of quaternion derivatives for cost functions (the so-called generalized $\mathbb{HR}$-calculus [21]). It explicitly reads

$$\hat{\boldsymbol{X}}_L = \boldsymbol{M} \cdot_L \boldsymbol{N}^{\mathsf{H}} \cdot_L \left(\boldsymbol{N} \cdot_L \boldsymbol{N}^{\mathsf{H}}\right)^{-1} . \tag{25}$$

To find the solution $\hat{\boldsymbol{X}}_R$ to (24), we first exploit the properties of left and right-sided matrix products such that $\|\boldsymbol{M} - \boldsymbol{X} \cdot_R \boldsymbol{N}\|_{\mathsf{F}}^2 = \|\boldsymbol{M}^{\mathsf{T}} - \boldsymbol{N}^{\mathsf{T}} \cdot_L \boldsymbol{X}^{\mathsf{T}}\|_{\mathsf{F}}^2$. Back to results provided in [20], we pose $\boldsymbol{Y} = \boldsymbol{X}^{\mathsf{T}}$ and obtain the minimizer as $\hat{\boldsymbol{Y}} = \left(\boldsymbol{N}^* \cdot_L \boldsymbol{N}^{\mathsf{T}}\right)^{-1} \cdot_L \boldsymbol{N}^* \cdot_L \boldsymbol{M}^{\mathsf{T}}$. Further simplifications yield:

$$\hat{\boldsymbol{X}}_R = \boldsymbol{M} \cdot_R \boldsymbol{N}^{\mathsf{H}} \cdot_R \left[\left(\boldsymbol{N}^* \cdot_L \boldsymbol{N}^{\mathsf{T}}\right)^{-1}\right]^{\mathsf{T}} . \tag{26}$$

5.2. Q-ALS for Q-CPD

Quaternion ALS (Q-ALS) is an iterative block coordinate optimization algorithm. After initialization, each iteration consists in computing the least squares updates of the factor matrices from the one obtained at the previous iteration. Using unfoldings (20)-(22) and the quaternion matrix least squares updates given in (23)-(24), the Q-ALS updates are given by:

$$\boldsymbol{A} \leftarrow \boldsymbol{T}_{(1)} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{B})^* \cdot_L \left((\boldsymbol{C} \odot_R \boldsymbol{B})^{\mathsf{T}} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{B})^*\right)^{-1}$$

$$\boldsymbol{B} \leftarrow \operatorname{Re}\left\{\boldsymbol{T}_{(2)} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{A})^* \cdot_L \left((\boldsymbol{C} \odot_R \boldsymbol{A})^{\mathsf{T}} \cdot_L (\boldsymbol{C} \odot_R \boldsymbol{A})^*\right)^{-1}\right\}$$

$$\boldsymbol{C} \leftarrow \boldsymbol{T}_{(3)} \cdot_R (\boldsymbol{B} \odot_R \boldsymbol{A})^* \cdot_R \left[\left((\boldsymbol{B} \odot_R \boldsymbol{A})^{\mathsf{H}} \cdot_L (\boldsymbol{B} \odot_R \boldsymbol{A})\right)^{-1}\right]^{\mathsf{T}} .$$

To obtain the $\boldsymbol{B}$-update, we solved the problem as if $\boldsymbol{B}$ was a quaternion matrix and projected the solution onto the reals.

6. NUMERICAL SIMULATIONS AND DISCUSSION

Numerical simulations aims at: *i)* demonstrating that the CPD can be computed in practice and *ii)* showing that the proposed algorithm behaves similarly to the real and complex ALS. We built 200 tensors of size $10 \times 10 \times 10$ according to (19) with $F = 4$ and Gaussian random i.i.d. factors matrices. We then added quaternion circular white Gaussian noise with prescribed signal to noise ratio (SNR). Q-ALS reconstruction performance was monitored using the relative mean-square error (rMSE) between estimated arrays and ground truth.

Fig. 1(a) plots the median value of the rMSE of estimated tensors and factor matrices. As expected, these values regularly decrease with the SNR. This shows that Q-ALS is relevant from a computational point of view. Its behavior seems similar to the standard ALS used for real/complex tensors. Fig. 1(b) shows that Q-ALS suffers from the same limitations as ALS: its performances decrease when the rank gets larger than tensor dimensions. This simulation uses noise-free tensors of size $5 \times 5 \times 5$ for varying rank values. This illustrates some of the research effort that must be made to devise efficient algorithms for the Q-CPD, and more generally, toward the design of new models and algorithms for the emerging field of quaternion tensors.

7. REFERENCES

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