Lower and upper bounds of quaternion tensor ranks

K.M.D.H. Kulathunga and Yang Zhang[0000-0002-0540-0893]

Department of Mathematics, University of Manitoba
Winnipeg, MB, R3T 2N2, Canada
kulatdhk@myumanitoba.ca; yang.zhang@umanitoba.ca

Abstract. Determining the tensor ranks is challenging, even for small-size tensors. Meanwhile, the tensor ranks may vary depending on the based fields. Up to now, most published results on the tensor ranks have been over the real/complex number fields or finite fields, which are commutative. A limited number of papers have been published on tensor ranks over non-commutative algebras. In this paper, we describe some properties of quaternion tensors, discuss the characterization of quaternion tensor ranks, and find the upper/lower bounds of the ranks for some quaternion tensors.

Keywords: Tensors· Rank · Quaternions.

1 Introduction

Quaternions (also called real quaternions or Hamilton quaternions) were discovered by William Rowan Hamilton in 1843. The set of quaternions is usually denoted by

$$\mathbb{H} = \{a + bi + cj + dk \mid i^2 = j^2 = k^2 = ijk = -1; a, b, c, d \in \mathbb{R}\}.$$

It is well known that $\mathbb{H}$ is a four-dimensional division algebra over the real field $\mathbb{R}$. Its applications can be traced back to 1890: Tait [37] expressed how quaternions were essential to the progress of physics in his book “On the Importance of Quaternions in Physics". Today, quaternionic quantum mechanics is one of the important branches in physics. Quaternions also have many applications in the current hot areas, such as robotics, dual-quaternion kinematics, computer vision, 3D registration, signal and image processing, and quaternion neural networks (see, e.g., [1, 10, 11, 26]). We refer the reader to [42] for detailed properties of $\mathbb{H}$.

A tensor is an algebraic object that consists of multidimensional arrays. It is most appropriate to refer to a tensor of size $(I_1, I_2, \ldots, I_K)$ as a K-way array or a K^{th}-order tensor. Generally, the set of K^{th}-order tensors of size $(I_1, I_2, \ldots, I_K)$ over an algebra $\mathbb{F}$ is denoted by $\mathbb{F}^{I_1 \times I_2 \times \ldots \times I_K}$ (see [21] for more details).

In matrix theory, a rank plays an important role and indicates the complexity of a matrix. The complexity of a tensor can be identified by its rank in a similar way. It is said that rank-one tensors are the simplest tensors which can be obtained by the tensor product of vectors. If we can decompose a tensor into the sum of rank-one tensors, then the minimum number of rank-one tensors needed to represent a tensor is known as the rank of a tensor.

Rank-one decomposition (also known as the polyadic form of a tensor) was first introduced by Hitchcock [14, 15] in 1927. Cattell [8,9] proposed the multiway model and the parallel proportional profile ideas in 1944, and Tucker [38,39] worked more on three-mode factor analysis in 1960. The rank-one decomposition was rediscovered several times, since it was not fully introduced until 1970. Carroll and Chang [7] introduced the CANDECOMP(canonical decomposition) form. Harshman [12] also introduced the PARAEAC(parallel factor analysis) form in the same year. The same decomposition has been explained in both papers. For the CANDECOM/PARAFAC model, Kiers [16] published standard notation and terminologies in 2000. Hence, this tensor decomposition is often referred to as CANDECOMP, PARAEAC, or CANDECOMP/PARAFAC(CP), which decomposes the tensors into the sum of rank-one tensors. The decomposition of a tensor into a minimum number of rank-one tensors is known as a tensor rank decomposition, minimal CP decomposition, or Canonical Polyadic Decomposition(CPD). In addition, there are many other tensor decompositions, such as Tucker decomposition and tensor train decomposition.

Unlike matrix rank, which can be computed efficiently, computing the rank of a higher-order tensor is NP-hard; indeed, deciding the tensor rank is NP-complete in general [13]. Hence, people are mostly working on determining the lower/upper bounds of the tensor ranks. Kruskal [18] showed several lower bounds for tensor ranks and certain conditions for the uniqueness of triple product factors of matrices in 1977. Atkinson and Stephens [3] investigated the number of non-scalar multiplications to consider a general family of bilinear forms in 1979. In addition, Atkinson and Lloyd [4, 5] studied upper bounds on the ranks of certain third-order tensors. They founded new limits considering matrix canonical forms and nonlinear strategies from commutative algebra in 1980 and considered the ranks for $m \times n \times (mn-2)$ tensors in 1983. It is shown that only one tensor with size $m \times n \times (mn-2)$ has rank $mn-1$, and others have rank at most $mn-2$ when the tensors with size $m \times n \times p$ with $p \leq mn-2$. Strassen [31] investigated the maximal border ranks for some tensors and the set of optimal bilinear computations for typical tensors in 1983.

After around 2000, more people joined to work on the tensor ranks. For example, Lathauwer et al.[22] proposed a multilinear generalization of the singular value decomposition. They investigated the effect of tensor symmetry on tensor decomposition and proposed a multilinear generalization of symmetric eigenvalue decomposition for pair-wise symmetric tensors. Kolda and Barder [17] published a survey paper on higher-order tensor decompositions and how they can be used in 2009. Landsberg [21] discussed the geometry and applications of tensors in 2012, and Lim [25] explored the properties and coordinate representations of tensors in 2014. Sumi et al.[32, 33, 34, 35, 36] provides more discussions. They determined the ranks of third-order tensors with two slices and Kronecker canonical forms, the maximal rank of third-order tensors, and the upper bounds of the ranks of order-n tensors with size $2 \times \cdots \times 2$. They considered all of this over the real and complex number field. Furthermore, typical ranks of $m \times n \times (m-1)n$ tensors have been determined over the real number field.

However, determining the tensor ranks is difficult even for small-size tensors. Moreover, the tensor ranks may vary on the based field. For example, the tensor ranks may be different for the cases of the real number field $\mathbb{R}$ and the complex number field $\mathbb{C}$. Numerous studies have been conducted for tensor decompositions and tensor ranks over the real/complex number fields. For example, [36] presents the maximal ranks of 3^{rd}-order tensors over the real and the complex number fields. The upper bounds for the ranks of tensors with size $2 \times \cdots \times 2$ over $\mathbb{R}$ and $\mathbb{C}$ have been studied in [34]. Furthermore, the maximal rank for any real $2 \times 2 \times 2 \times 2$ tensor is 5, while the maximal rank for a complex tensor of the same size is 4, which Kong and Jiang showed in [19] and Brylinski in [6], respectively. All of the above motivates us to discuss the ranks of quaternion tensors.

Calculating a minimal decomposition into rank-one tensors is not only theoretically beneficial, but also really important in real-world applications. Credit goes to Appellof and Davidson [2] for first applying the tensor decomposition in Chemometrics. Most recently, quaternion tensors have been successfully applied in color image processing. A quaternion tensor model for a color image treats the RGB channels as a single coupled object rather than three separate real-valued arrays. Then an image or video is organized as a quaternion matrix or higher-order quaternion tensor. This is attractive because it preserves cross-channel correlation and geometric/color structure that can be weakened when channels are processed in usual encoding independently (see, e.g. [27–30, 40, 43]). This is another motivation for us to consider the rank of quaternion tensors.

2 Definitions and main results

A nonzero Kth-order quaternion tensor $\mathscr{X}$ is called a rank-one tensor if $\mathscr{X}$ can be written as the outer product of the K vectors, i.e.,

$$\mathscr{X} = \overrightarrow{\mathrm{v_1}} \otimes \overrightarrow{\mathrm{v_2}} \otimes \cdots \otimes \overrightarrow{\mathrm{v_K}},$$

where $\overrightarrow{\mathrm{v_1}} = (v_{11}, v_{12}, \ldots, v_{1I_1}), \ldots, \overrightarrow{\mathrm{v_K}} = (v_{K1}, v_{K2}, \ldots, v_{KI_K})$. Thus, each element of the quaternion tensor is the product of the related vector elements:

$$(\mathscr{X}_{i_1 i_2 \cdots i_K}) = (v_{1i_1} v_{2i_2} \cdots v_{Ki_K})$$

Definition 1. *Let $\mathscr{X}$ be a nonzero K^{th}-order quaternion tensor. Then the rank of $\mathscr{X}$ is the smallest positive integer n such that $\mathscr{X} = \mathscr{X}_1 + \mathscr{X}_2 + \cdots + \mathscr{X}_n$, where $\mathscr{X}_1, \mathscr{X}_2, \ldots, \mathscr{X}_n$ are rank-one K^{th}-order tensors. We will say that $\mathscr{X}$ has rank n, denoted by $rank(\mathscr{X}) = n$.*

The challenge is the non-commutativity of quaternions, which makes many methods that are valid on real/complex numbers invalid on quaternions. In particular, the rank of a quaternion matrix may vary after using row and column operations since quaternions are non-commutative. For example, consider the matrix $M = \begin{bmatrix} i+5j & i+5j \\ 2+i-k & 2+i-k \end{bmatrix}$. Clearly, rank$(M) = 1$. Now, we apply the following two-column operations to M and obtain:

$$M = \begin{bmatrix} i+5j & i+5j \\ 2+i-k & 2+i-k \end{bmatrix} \xrightarrow[C_2 \to C_2 i]{C_1 \to iC_1} \begin{bmatrix} -1+5k & -1-5k \\ -1+2i+j & -1+2i-j \end{bmatrix} = N.$$

It is easy to check rank$(N) = 2$. That is, the rank of the matrix M has increased with the column operations.

The rank is preserved for the quaternion matrix only when applying left-row operations (multiplying the corresponding row by the corresponding quaternion number on the left) and right-column operations (multiplying the corresponding column by the corresponding quaternion number on the right). Those are called rank-preserving operations. Using this operation, we prove the following upper boundary theorem.

Theorem 1. *Let $\mathscr{X} \in \mathbb{H}^{I_1 \times \cdots \times I_K}$. Then*

$$rank(\mathscr{X}) \leq max.rank\ of\ \mathbb{H}^{I_1 \times \cdots \times I_k} \left(\prod_{i=k+1}^{K} I_i \right),\ 1 \leq k \leq K.$$

The process of rearranging the elements of a Kth-order quaternion tensor into a quaternion matrix is called flattening of quaternion tensors (also called matricization or unfolding), which is an important technique. In particular, it is quite efficient for the three-order tensors. For quaternion tensors in $\mathbb{H}^{I_1 \times I_2 \times I_3}$, it is important to note that we adopt the convention where I_1 denotes the number of horizontal slices, I_2 the number of frontal slices and I_3 the number of lateral slices. In such a way, we can handle quaternion row/column transformations more efficiently. This is different from that used by the papers in the commutative case.

In [23, 24], we have provided a full classification of the maximum ranks of third-order quaternion tensors $\mathbb{H}^{I_1 \times I_2 \times I_3}$ with $1 \leq I_i \leq 3$. In this section, we discuss more general cases.

For an $m \times n$ quaternion matrix M, a unique expression can be written as follows: $M = M_1 + M_2 j$, where M_1 and M_2 are $m \times n$ matrices with entries in $\mathbb{C}$. The complex adjoint matrix of M (or simply the adjoint matrix of M) is defined as the complex block matrix of $2m \times 2n$,

$$\mathcal{X}_M = \begin{pmatrix} M_1 & M_2 \\ -\overline{M_2} & \overline{M_1} \end{pmatrix}.$$

An $n \times n$ quaternion matrix M is diagonalizable if and only if $\mathcal{X}_M$ is diagonalizable. Using this representation and other properties, we obtain the following results for quaternion tensors. The first two results are about the lower boundary of quaternion tensors under some conditions.

Theorem 2. *Let $\mathscr{X} \in \mathbb{H}^{p\times q\times r}$ and write $\mathscr{X} = (M_1; \ldots; M_r)$, where $M_1, \ldots, M_r$ are $p \times q$ quaternion matrices. Then*

$$rank(\mathscr{X}) \geq max\{rank(d_1M_1; \ldots; d_rM_r) \mid d_1, \ldots, d_r \in \mathbb{R}\}.$$

Theorem 3. *Let $\mathscr{X} \in \mathbb{H}^{q\times(p-1)q\times p}$ and $\mathscr{X} = (M_1; M_2; \ldots; M_p)$, where $M_1 = (I_q, 0_{q\times(p-2)q})$, $M_2 = (0_{q\times q}, I_q, 0_{q\times(p-3)q}), \ldots, M_{p-1} = (0_{q\times(p-2)q}, I_q), M_p = (Y_1, Y_2, \ldots, Y_{p-1})$, and I_q is an identity matrix. Suppose that any nontrivial linear combination of $Y_1, Y_2, \ldots,$ Y_{p-1}, I_q is non-singular. Then $rank(\mathscr{X}) > (p-1)q$.*

The following theorem gives an exact maximum rank for one case. It is worth pointing out that this theorem might not be true if the order of the indices is changed.

Theorem 4. *Let $\mathscr{X} \in \mathbb{H}^{p\times q\times(pq-r)}$ be with $r \leq min(p, q)$. Then*

$$max.rank\ of\ \mathscr{X} = pq - r^2 + max.rank\ of\ \mathscr{Y},\ \mathscr{Y} \in \mathbb{H}^{r\times r\times(r^2-r)}.$$

In general, we have the following rough estimate. For some cases, we can construct examples to reach the maximum ranks.

Theorem 5. *The upper bound of the maximum rank of quaternion tensors with size $p \times q \times r$ is the minimum of $\{pq, pr, qr\}$.*

The proofs of Theorems 1 to 5 and more results can be found in [20].

3 Maple package for quaternion tensors

To our best knowledge, there is no standard Maple package in Maple's official documentation or Application Center. There are Maple worksheets/packages for ordinary Hamilton quaternions. For example, Maplesoft's Application Center has quaternion examples, and David Harder's Quaternions Maple package allows users to work with quaternions more naturally in Maple.

Maple also has built-in tensor tools, especially through DifferentialGeometry[Tensor]. These are mainly for differential geometry/tensor calculus, not numerical quaternion tensor decompositions such as quaternion tensor SVD, QR, t-product, tensor rank, etc. In our previous work [23, 24], we have used our own Maple commands to classify the ranks of all $p \times q \times r$ $(1 \leq p, q, r \leq 3)$ third-order quaternion tensors.

The most recent quaternion-tensor work is implemented in MATLAB/Python-style numerical frameworks, not in a standard Maple package.

All of the above motivates us to design a Maple package, `QuaternionTensor,` for symbolic and numerical experiments with quaternion matrices/tensors.

In this Maple implementation, we used `Q(a,b,c,d)` to create a quaternion $q = a+bi+cj+dk$ and represented it by the list $[a, b, c, d]$ of real numbers. Quaternion arithmetic is implemented through `QAdd` (addition), `QSub` (subtraction), `QMul` (multiplication), `QInverse` (inverse), `QEqual` (equal), `QConj` (conjugate), `QNormSq` (Frobenius norm), and others. For example, the Maple commands for a quaternion $1 + 2i + 3j + 4k$ and others produce:

```
q := Q(1,2,3,4);
         [1, 2, 3, 4]
QNormSq(Q(1,2,3,4));
             30
QMul(Q(1,2,3,4),Q(5,6,7,8));
         [-60.12.30.24]
QConj(Q(1,2,3,4));
         [1,-2,-3,-4]
```

A quaternion matrix is a Maple command `Matrix` whose entries are such four-component lists, and a third-order quaternion tensor $\mathscr{X} \in \mathbb{H}^{p\times q\times r}$ is represented as a list of frontal slices $\mathscr{X} = [M_1, M_2, \ldots, M_r]$, where each M_k is a $p \times q$ quaternion matrix.

The rank of the quaternion matrix is computed using the standard complex adjoint representation. If $M = M_1 + M_2 j$, where $M_1 = A + Bi$, $M_2 = C + Di$, and A, B, C, D are real matrices, then the code constructs

$$\chi_M = \begin{bmatrix} M_1 & M_2 \\ -\overline{M_2} & \overline{M_1} \end{bmatrix}.$$

The function `ComplexAdjoint(M)` returns this complex matrix, and the rank command `QuaternionMatrixRank(M)` returns $\frac{1}{2}\,\mathrm{rank}_{\mathbb{C}}(\chi_M)$. For example,

```
A:= Matrix(2, 2,[[[1,0,-1,2],[-2,1,0,0]],[[0,2,1,-1],[1,-2,2,0]]]);
QuaternionMatrixRank(A);
B:= ComplexAdjoint(A);
```

$$A := \begin{bmatrix} [1,0,-1,2] & [-2,1,0,0] \\ [0,2,1,-1] & [1,-2,2,0] \end{bmatrix}$$

$$2$$

$$B := \begin{bmatrix} 1 & -2+I & -1+2I & 0 \\ 2I & 1-2I & 1-I & 2 \\ 1+2I & 0 & 1 & -2-I \\ -1-I & -2 & -2I & 1+2I \end{bmatrix}$$

The package contains three random generation functions: `RandomQuaternion, RandomQMatrix, RandomQTensor`.

The command `RandomQuaternion(range)` generates a random quaternion $q = [a, b, c, d] = a + bi + cj + dk$, where the four components a, b, c, d are sampled independently from the discrete uniform distribution on the integer values in `range`. The default range is $-5..5$. Similarly, `RandomQMatrix(p,q,range)` and `RandomQTensor(p,q,r,range)` generate random quaternion $p\times q$ matrices and $p\times q\times r$ tensors with independent entries from this distribution. For example,

```
RandomQTensor(2, 2, 3, -4 .. 4);
```

$$\left[\begin{bmatrix} [4,0,-2,-4] & [4,3,2,-2] \\ [2,-2,3,-1] & [-4,2.-4,1] \end{bmatrix}, \begin{bmatrix} [3,-1,-4,-1] & [-2,-3,1,-4] \\ [1,2,-4,-3] & [4,3,-4,2] \end{bmatrix},\right.$$
$$\left.\begin{bmatrix} [2,0,-2,0] & [0,-2,-1,4] \\ [0,2,0,-4] & [1,4,-4,-2] \end{bmatrix}\right]$$

generates a third-order tensor in $\mathbb{H}^{2\times 2\times 3}$, represented as a list of 3 frontal slices which are 2×2 matrices.

For a tensor $\mathscr{X} \in \mathbb{H}^{p\times q\times r}$, the package computes three matrix unfoldings: `FlattenMode1(X)`, `FlattenMode2(X)`, and `FlattenMode3(X)`. Their sizes are $X_1 \in \mathbb{H}^{p\times qr}$, $\quad X_2 \in \mathbb{H}^{q\times pr}$, $\quad X_3 \in \mathbb{H}^{r\times pq}$.

`FlatteningRanks(X)` returns their quaternion matrix ranks as a list below:

```
[rank(FlattenMode1(X)),rank(FlattenMode2(X)),rank(FlattenMode3(X))]
```

These ranks provide lower bounds for the tensor rank. Since every rank-one quaternion tensor has matrix rank at most one in each flattening,

$$\mathrm{rank}_{\mathbb{H}}(\mathscr{X}) \geq \max\left\{\mathrm{rank}_{\mathbb{H}}(X_1), \mathrm{rank}_{\mathbb{H}}(X_2), \mathrm{rank}_{\mathbb{H}}(X_3)\right\}.$$

The function `LowerBoundTheorem2(X, samples=20, range=-5..5)` implements the lower-bound idea based on real linear combinations of frontal slices in Theorem 2. If $\mathscr{X} = [M_1, M_2, \ldots, M_r]$, then the function considers matrices of the form

$$M(d) = d_1 M_1 + d_2 M_2 + \cdots + d_r M_r,$$

where $d_1, \ldots, d_r \in \mathbb{R}$. It computes the quaternion matrix rank of several such matrices and returns the largest rank found. The coefficient vectors include:

(i) the standard coordinate vectors $e_1, \ldots, e_r$,
(ii) the all-ones vector $(1, 1, \ldots, 1)$, and
(iii) additional random integer coefficient vectors.

The default random coefficients are sampled independently from $\{-5, \ldots, 5\}$. Therefore, the default command uses discrete uniform random coefficients in the range `-5..5`. The returned value is a valid lower bound based on the tested coefficient vectors, but it is not necessarily the exact maximum over all real coefficients.

The function `UpperBoundTheorem5(p,q,r)` returns the theoretical upper bound $\min\{pq, pr, qr\}$ in Theorem 5.

The function `RankOneTensor(u,v,w)` constructs a rank-one quaternion tensor with entries $x_{ijk} = u_i v_j w_k$. For example,

```
u := [Q(1,0,0,0), Q(0,2,0,0)]:
v := [Q(3,0,0,0), Q(0,0,4,0)]:
w := [Q(5,0,0,0), Q(0,0,0,6)]:
X := RankOneTensor(u,v,w);
```

$$X := \left[\begin{bmatrix} [15,0,0,0] & [0,0,20,0] \\ [0,30,0,0] & [0,0,0,40] \end{bmatrix}, \begin{bmatrix} [0,0,0,18] & [0,24,0,0] \\ [0,0,-36,0] & [-48,0,0,0] \end{bmatrix}\right]$$

constructs a tensor in $\mathbb{H}^{2\times 2\times 2}$, represented as two 2×2 frontal slices.

The function `CPReconstruct(terms)` takes a list of rank-one terms and adds them together. Therefore, if `terms` contains n rank-one terms, then the reconstructed tensor has rank at most n.

The function `ResidualNormSq(X,Y)` computes the squared Frobenius-type residual norm of tensors

$$\|\mathscr{X} - \mathscr{Y}\|_F^2 = \sum_{i,j,k} |x_{ijk} - y_{ijk}|^2.$$

If $\mathscr{Y}$ is an exact reconstruction of $\mathscr{X}$, then `ResidualNormSq(X,Y)` returns 0.

There is no explicit numerical threshold used in the current code for this paper. Since the default random entries are exact integers, we applied Maple's exact `LinearAlgebra:-Rank` function to the complex adjoint matrix. Therefore the rank is computed symbolically/exactly. If floating-point entries are used, then a numerical singular-value threshold should be introduced. A common numerical rule is $\mathrm{rank}(A) = \#\{\sigma_i(A) > \varepsilon\}$, where $\sigma_i(A)$ are the singular values of a complex matrix A. A typical fixed threshold is $\varepsilon = 10^{-10}$, or a scale-dependent threshold such as $\varepsilon = 10^{-10}\sigma_{\max}(A)$. For a quaternion matrix M, this would give

$$\mathrm{rank}_{\mathbb{H}}(M) = \frac{1}{2}\#\{\sigma_i(\chi(M)) > \varepsilon\}.$$

This package also includes quaternion tensor decompositions such as QR, LU and SVD, and solving quaternion tensor equations, which are related to our other works (see, e.g., [41, 44]). On the other hand, we are developing Maple packages for split quaternion tensors and reduced biquaternions tensors. Our final goal is to build a standard Maple package for quaternions, split quanternions, reduced biquaternions, and matrices/tensors over them.

Maple codes are available upon request and can be downloaded from https://umanitoba.ca/science/directory/mathematics/yang-zhang.

Acknowledgments. The author would like to thank the Editors and anonymous referees for their valuable comments. This study was funded by Canada NSERC (RGPIN 2020-06746).

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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