

Trace Invariance for Quaternion Matrices

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ABSTRACT

Let F be a field. It is a classical result in linear algebra that for each $A, P \in M_n(F)$ such that P is nonsingular, $\text{tr } A = \text{tr } (PAP^{-1})$. We show in this paper that the preceding property does not hold true if F is the division ring of real quaternions. We show that the only quaternion matrices that have their trace invariant under unitary similarity are Hermitian matrices, and that the only matrices that have their trace invariant under similarity are real scalar matrices.

Keywords: Trace, quaternion, unitary matrices, Hermitian matrices

LAYMAN'S ABSTRACT

We consider a classical result in linear algebra concerning the trace of matrices with complex entries and we determine whether this result holds true for the set of quaternion matrices.

INTRODUCTION

The trace of a square matrix A , $\text{tr}(A)$, is the sum of the diagonal entries of A . If the entries of A come from the field \mathbb{C} of complex numbers, then $\text{tr}(A)$ is a linear functional and is used to define the inner product $(A, B) = \text{tr}(B^*A)$ on $M_n(\mathbb{C})$. Trace is studied in the literature in different contexts. Heunen and Horsman (2013) studied the trace in relation to orthogonality of vectors. Xiang et al. (2013) provided trace minimizing properties of certain positive semidefinite matrices. Mckee and Yatsyna (2014) studied the trace of connected integer symmetric matrices. Wang and Zhu (2013) studied the trace of elements of modular groups. The trace is also of particular interest in Terwilliger algebras (Kang et al. 2004; Nomura and Terwilliger 2006).

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It is routine to show that if A and B are n -by- n matrices with entries from a field F , then $\text{tr}(AB) = \text{tr}(BA)$. In particular, the trace is invariant under similarity, that is, if $A, P \in M_n(F)$ with P nonsingular, then $\text{tr}(PAP^{-1}) = \text{tr}(A)$. We show that if A is an n -by- n matrix with quaternion entries, then $\text{tr}(PAP^{-1}) = \text{tr}(A)$ for all nonsingular P if and only if A is a real scalar matrix. We also show that $\text{tr}(UAU^{-1}) = \text{tr}(A)$ for all unitary U if and only if A is Hermitian.

RESULTS AND DISCUSSION

Preliminaries

We denote the set of all quaternions over the field \mathbb{R} of real numbers by \mathbb{H} , that is, $\mathbb{H} = \{a + bi + cj + dk \mid a, b, c, d \in \mathbb{R}\}$, where $ijk = i^2 = j^2 = k^2 = -1$. Let $x = a + bi + cj + dk$, where $a, b, c, d \in \mathbb{R}$. The real part of x is a , the i part of x is b , the j part of x is c , and the k part of x is d . The set \mathbb{H} , which contains the complex numbers, is of interest in many fields of mathematics and physics (Grigoryan et al. 2015; Li and Bai 2015; Shao 2015; Wang et al. 2015). Let \mathbb{S} be \mathbb{R} , \mathbb{C} , or \mathbb{H} . We denote by $M_{m,n}(\mathbb{S})$ the set of all m -by- n matrices with entries from \mathbb{S} . We also write $M_n(\mathbb{S}) = M_{n,n}(\mathbb{S})$. The set \mathbb{S}^n denotes the set of n -by-column vectors with entries from \mathbb{S} .

For $a = a_1 + a_2i + a_3j + a_4k \in \mathbb{H}$, the (quaternion) conjugate of a is $\bar{a} \equiv a_1 - a_2i - a_3j - a_4k$. The (quaternion) modulus of a , denoted by $|a|$,

is $|a| \equiv \sqrt{aa}$. One checks that $|a| = \sqrt{aa} = \sqrt{a_1^2 + a_2^2 + a_3^2 + a_4^2} = \sqrt{a\bar{a}} = |\bar{a}|$. Observe that if $a \in \mathbb{C}$, then the (quaternion) conjugate and the (quaternion) modulus of a are just the usual conjugate and modulus of a . We observe that if

$a \in \mathbb{H}$ is nonzero, then the multiplicative inverse of a is $a^{-1} = \frac{\bar{a}}{|a|^2}$.

The symbols A^T , A , and A^* denote the transpose, conjugate, and the conjugate transpose of a matrix A , respectively. An $A \in M_n(\mathbb{H})$ is left (right) nonsingular if there exists a matrix $B \in M_n(\mathbb{H})$ such that $BA = I$ ($AB = I$). Zhang (1997) has shown that for $A, B \in M_n(\mathbb{H})$, we have $(AB = I)$ if and only if $BA = I$. Hence, a matrix A is left nonsingular if and only if it is right nonsingular. We refer to a left or right nonsingular matrix as nonsingular. It is also known that if B exists, then B is unique, and we call B the (quaternion) inverse of A (denoted $B = A^{-1}$). We note that the usual properties of complex inverses also hold for the quaternion inverse: $(A^{-1})^{-1} = A$ and $(AB^{-1})^{-1} = B^{-1}A^{-1}$. Thus, the set of n -by- n nonsingular quaternion matrices forms a

group under multiplication. Like in the complex case, we say that two matrices $A, B \in M_n(\mathbf{H})$ are (quaternion) similar if there exists a nonsingular such that $PAP^{-1} = B$.

Let $A \in M_n(\mathbf{H})$ and write $A = A_1 + A_2j$, where $A_1, A_2 \in M_n(\mathbf{C})$. The complex partition of A (Zhang 1997) is the $2n$ -by- $2n$ complex matrix $\chi_A = \begin{bmatrix} A_1 & A_2 \\ -A_2 & A_1 \end{bmatrix}$.

The complex partition of A , also called the complex adjoint of A , is used to prove that if $A, B \in M_n(\mathbf{H})$, then $AB = I$ if and only if $BA = I$ (Zhang 1997). The complex partition is also used in the study of the numerical range in quaternionic Hilbert spaces (Au-Yeung 1984). We observe that $\text{tr } \chi_A = \text{tr } A_1 + \text{tr } A_1 = 2\text{Re}(\text{tr } A)$. Zhang (1997) has identified the following (Theorem 4.2 (2) and (5)).

Proposition 1. Let $A, B \in M_n(\mathbf{H})$. Then $\chi_A \chi_B = \chi_{AB}$. Moreover, if A is non-singular, then χ_A is nonsingular and $(\chi_A)^{-1} = \chi_{A^{-1}}$.

Let $E_{ij} \in M_n(\mathbf{H})$ be the matrix having 1 as its (i, j) -entry and zero for the other entries.

Let U_n denote the set of all n -by- n unitary quaternion matrices, that is, matrices $U \in M_n(\mathbf{H})$ satisfying $UU^* = I_n$. A matrix $A \in M_n(\mathbf{H})$ is said to be nilpotent if there exists a positive integer m such that $A^m = 0$.

Let $a, b \in \mathbf{H}$. We say that a is similar to b if there exists a nonzero $x \in \mathbf{H}$ such that $xax^{-1} = b$. Observe that $xy \neq yx$ in general, but xy is always similar to yx (if at least one of x or y is 0, then $xy = yx$; otherwise, $y(xy)^{-1} = yx$; and that $xax^{-1} = a$ for all nonzero $x \in \mathbf{H}$ if and only if $a \in \mathbf{R}$). Let $A \in M_n(\mathbf{H})$ and $x \in \mathbf{H}^n$ be nonzero. If $Ax = x\lambda$ ($Ax = \lambda x$) for some $\lambda \in \mathbf{H}$, then we say that λ is a right (left) eigenvalue of A . We observe that since multiplication in \mathbf{H} is not commutative, the left and right eigenvalues of A may be different. In this paper, we call the right eigenvalues of A the eigenvalues of A . It is easy to see that similar quaternion matrices have the same set of eigenvalues. In particular, it is known that an n -by- n quaternion matrix has exactly n complex eigenvalues. We call these the standard eigenvalues of A . It is also known that all other eigenvalues of A are similar to the standard eigenvalues of A (Zhang 1997). Thus, if the standard eigenvalues of A are real, then the eigenvalues of A are the standard eigenvalues of A . We denote by $\sigma(A)$ the collection of all eigenvalues of A .

Zhang (1997) has outlined the other properties of \mathbf{H} and $M_n(\mathbf{H})$.

Trace Invariance Under Similarity

We study the trace of a matrix over the ring of quaternions. We begin with the following.

Remark 2. There exist $A, B \in M_n(\mathbb{H})$ and nonsingular $P \in M_n(\mathbb{H})$ such that $PAP^{-1} = B$ and $\text{tr}(A) \neq \text{tr}(B)$.

We give the following as an example. If $A = \begin{bmatrix} k & 0 \\ 0 & -k \end{bmatrix}$ and $B = \begin{bmatrix} -k & 0 \\ 0 & -k \end{bmatrix}$, then $\begin{bmatrix} i & 0 \\ 0 & k \end{bmatrix} A \begin{bmatrix} -i & 0 \\ 0 & -k \end{bmatrix} = B$. Thus A is (unitarily) similar to B but $\text{tr} A = 0 \neq -2k = \text{tr} B$.

We ask when is it possible for the trace to be invariant under similarity or what properties of the trace in the complex case are still applicable to the quaternion case. We start with the following proposition.

Proposition 3. For each $A, P \in M_n(\mathbb{H})$ with P nonsingular, $\text{Re}(\text{tr}(A)) = \text{Re}(\text{tr}(PAP^{-1}))$.

Proof. Let $A, P \in M_n(\mathbb{H})$ such that P is nonsingular and $B = PAP^{-1}$. Note that $\text{tr}(\chi_A) = 2\text{Re}(\text{tr}(A))$ and $\text{tr}(\chi_B) = 2\text{Re}(\text{tr}(PAP^{-1}))$. By Proposition 1 $\chi_B = \chi_{PAP^{-1}} = \chi_P \chi_A \chi_{P^{-1}} = \chi_P \chi_A \chi_P^{-1}$. Hence $\text{tr}(\chi_B) = \text{tr}(\chi_A)$ and so $\text{Re}(\text{tr}(A)) = \text{Re}(\text{tr}(PAP^{-1}))$.

The following corollary is a consequence of Proposition 3 and the fact that if $A \in M_n(\mathbb{H})$ is Hermitian ($A^* = A$), then $\text{tr}(A) \in \mathbb{R}$. We recall that for $A, B \in M_n(\mathbb{H})$, $(AB)^* = B^* A^*$ and so the set of Hermitian quaternion matrices is closed under unitary similarity.

Corollary 4. Let $A \in M_n(\mathbb{H})$ be Hermitian. Then $\text{tr}(A) = \text{tr}(UAU^{-1})$ for all $U \in \mathbb{U}_n$.

We ask if the converse of Corollary 4 is true. Before we answer that, we observe the following.

Proposition 5. Let $A \in M_n(\mathbb{H})$. If for every $U \in \mathbb{U}_n$, $\text{tr}(A) = \text{tr}(UAU^{-1})$, then the diagonal entries of A are real.

Proof. Let $A = [a_{ij}] \in M_n(\mathbb{H})$. Suppose for all $U \in \mathbb{U}_n$, $\text{tr}(A) = \text{tr}(UAU^{-1})$. Suppose that $a_{pp} = a \notin \mathbb{R}$ for some $p \in \{1, \dots, n\}$, then there exists $v \in \mathbb{H}$ such that $va v^{-1} \neq a$. Moreover we can take v to have modulus 1 so that $v^{-1} = \bar{v}$. We then consider WAW^{-1} , where W is the unitary diagonal matrix having v as its p th diagonal entry, and 1 as its other diagonal entries. We see that $\text{tr}(WAW^{-1}) = \text{tr}(A) - a + va v^{-1} \neq \text{tr}(A)$, which is a contradiction. Therefore all diagonal entries of A are real.

Corollary 6. Let $A \in M_n(\mathbb{H})$. If for every $U \in \mathbf{U}_n$, we have $\text{tr}(A) = \text{tr}(UAU^{-1})$, then $\text{tr}(A) \in \mathbb{R}$.

Zhang (1997) has identified the following as Theorems 6.1 and 6.2.

Theorem 7. Let $A \in M_n(\mathbb{H})$. There exists $V \in \mathbf{U}_n$ such that VAV^{-1} is upper triangular. If A is upper triangular, then every diagonal entry of A is an eigenvalue of A . Conversely, every eigenvalue of A is similar to a diagonal entry of A .

Theorem 8. Let $A \in M_n(\mathbb{H})$ and $\lambda \in \sigma(A)$. There exists a unitary U such that UAU^* is upper triangular and λ is a diagonal entry of UAU^* .

Proof. Let $A \in M_n(\mathbb{H})$ and $\lambda \in \sigma(A)$. By Theorem 7, there exists $V_1 \in \mathbf{U}_n$ such that $B \equiv V_1AV_1^{-1} = [b_{ij}]$ is upper triangular, and there exists an index p such that the p th diagonal entry of B is similar to λ , say $\lambda = vb_{pp}v^{-1}$. Note also that we may assume without loss of generality that v has modulus 1. Let $V_2 = I_{p-1} \oplus vI_1 \oplus I_{n-p}$ and observe that $V_2 \in \mathbf{U}_n$. $C \equiv V_2V_1A(V_2V_1)^{-1}$ is upper triangular such that the p th diagonal entry of C is λ , as desired.

Corollary 9. Let $A \in M_n(\mathbb{H})$. If $\text{tr}(A) = \text{tr}(UAU^{-1})$ for every $U \in \mathbf{U}_n$, then $\sigma(A) \subset \mathbb{R}$.

Proof. Let $A \in M_n(\mathbb{H})$ and $\lambda \in \sigma(A)$. Suppose $\text{tr}(A) = \text{tr}(UAU^{-1})$ for every $U \in \mathbf{U}_n$. Let $V \in \mathbf{U}_n$ such that $B \equiv VAV^{-1}$ is upper triangular and λ is a diagonal entry of B . Then for every $U \in \mathbf{U}_n$, we have $\text{tr}(B) = \text{tr}(UBU^{-1})$. Hence, by Proposition 5, B has real diagonal entries, and so $\sigma(A) \subset \mathbb{R}$.

The converses of Corollary 6 and of Corollary 9 are not always true. Take $A = \begin{bmatrix} i & j \\ -j & i \end{bmatrix}$,

then $A^2 = 0$ and so there exist a unitary U and $b > 0$ such that $UAU^{-1} = bE_{12}$ (Merino and Sergeichuk 1999, Theorem 5). Note that bE_{12} is a matrix having real diagonal entries and real eigenvalues but $\text{tr}(bE_{12}) = 0 \neq 2i = \text{tr}(A)$.

We now look into the converse of Corollary 4. We first prove the following lemma.

Lemma 10. For each $a \in \mathbb{R}$ and $U \in \mathbf{U}_n$, we have $\text{tr}(aE_{rr}) = \text{tr}(U(aE_{rr})U^{-1})$ for each $1 \leq r \leq n$.

Proof. Let $a \in \mathbb{R}$, let $U = [u_{st}] \in \mathbf{U}_n$ and let $1 \leq r \leq n$. Then $U^*U = I$ implies that $\sum_{p=1}^n \overline{u_{pr}} u_{pr} = \sum_{p=1}^n \overline{u_{pr}} u_{pr} = 1$. One computes that $\text{tr}(U(aE_{rr})U^{-1}) = \sum_{p=1}^n \overline{u_{pr}} a u_{pr} = a \sum_{p=1}^n \overline{u_{pr}} u_{pr} = a$.

If $D = \text{diag}(d_1, d_2, \dots, d_n)$, then $D = \sum_{i=1}^n d_i E_{ii}$. Thus, the following holds by Lemma 10.

Corollary 11. For each diagonal $D \in M_n(\mathbb{R})$ and $U \in U_n$, we have that $\text{tr}(D) = \text{tr}(UDU^{-1})$.

Lemma 12. Let $0 \neq A \in M_n(\mathbb{H})$ be nilpotent. Then there exists $T \in U_n$ such that $\text{tr}(TAT^{-1})$ is nonzero.

Proof. Let $0 \neq A \in M_n(\mathbb{H})$ be nilpotent. Let such $V \in U_n$ that VAV^{-1} is upper triangular. Since A is nilpotent, the diagonal entries of VAV^{-1} are all 0. Since $A \neq 0$, VAV^{-1} has a nonzero (s, t) entry for some $s < t$. Write the (s, t) nonzero entry of VAV^{-1} as $b = b_1 + b_2i + b_3j + b_4k$. We show that there exists a unitary T such that $\text{tr}(TAT^{-1})$ is nonzero for the case when $b_2 \neq 0$. Similar arguments can be used to show that a similar conclusion holds if b_3 or b_4 is nonzero. Take

$$X = \frac{1}{\sqrt{2}} \begin{bmatrix} I_{s-1} & 0 & 0 & 0 & 0 \\ 0 & k & 0 & 1 & 0 \\ 0 & 0 & I_{t-1-s} & 0 & 0 \\ 0 & 1 & 0 & k & 0 \\ 0 & 0 & 0 & 0 & I_{n-t} \end{bmatrix} \quad (1)$$

which gives us

$$X^{-1} = \frac{1}{\sqrt{2}} \begin{bmatrix} I_{s-1} & 0 & 0 & 0 & 0 \\ 0 & -k & 0 & 1 & 0 \\ 0 & 0 & I_{t-1-s} & 0 & 0 \\ 0 & 1 & 0 & -k & 0 \\ 0 & 0 & 0 & 0 & I_{n-t} \end{bmatrix} \quad (2).$$

One computes that $\text{tr}(XVA(XV)^{-1}) = -(b_3i - b_2j)$ which is nonzero when b_2 is nonzero. Now, assume that $b_1 \neq 0$ and $b_2 = b_3 = b_4 = 0$. Without loss of generality, we assume that b_1 is positive, since otherwise, we consider $-VAV^{-1}$. Recall that there is a nonsingular X_1 such that $X_1^{-1} \begin{bmatrix} i & j \\ -j & i \end{bmatrix} X_1 = \begin{bmatrix} 0 & b_1 \\ 0 & 0 \end{bmatrix}$ for some positive b . Let

$$X_1 = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix} \quad \text{and let } X = \begin{bmatrix} I_{s-1} & 0 & 0 & 0 & 0 \\ 0 & x_{11} & 0 & x_{12} & 0 \\ 0 & 0 & I_{t-1-s} & 0 & 0 \\ 0 & x_{21} & 0 & x_{22} & 0 \\ 0 & 0 & 0 & 0 & I_{n-t} \end{bmatrix}.$$

One computes that $\text{tr}(XVA(XV)^{-1}) = 2i$, which is nonzero. For all the cases, we take $T = XV$ as the desired unitary matrix.

Theorem 13. Let $A \in M_n(\mathbb{H})$. Then $\text{tr}(A) = \text{tr}(UAU^{-1})$ for every unitary U if and only if A is Hermitian.

Proof. Sufficiency is already proved in Corollary 4. For the forward implication we consider $U \in \mathbf{U}_n$ such that $B = UAU^{-1}$ is upper triangular. By Corollary 9, B has real diagonal entries. Now, suppose A is not Hermitian. Then we can write $B = D + N$ where D is a real diagonal matrix, $\text{tr}(D) = \text{tr}(B) = \text{tr}(A)$, and N is a strictly upper triangular nonzero nilpotent matrix. Lemma 12 guarantees that there exists a unitary T such that TNT^{-1} has nonzero trace. But $\text{tr}(TDT^{-1}) = \text{tr}(D)$ by Corollary 11, and so we get $0 = \text{tr}(B) - \text{tr}(D) = \text{tr}(TBT^{-1}) - \text{tr}(TDT^{-1}) = \text{tr}(TNT^{-1}) \neq 0$, which is a contradiction. Hence A is Hermitian.

We then ask if $A \in M_n(\mathbb{H})$ being Hermitian is sufficient for the trace to be invariant under similarity in general. One observes that the answer to the preceding is yes

for the case when $n = 1$. However, if $n > 1$, $A = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \oplus 0_{n-2}$, and $P = \begin{bmatrix} 1 & i+k \\ -(i+k) & 0 \end{bmatrix} \oplus I_{n-2}$ then A is Hermitian, P is nonsingular with $P^{-1} = \begin{bmatrix} 0 & \frac{i+k}{2} \\ \frac{-(i+k)}{2} & \frac{1}{2} \end{bmatrix} \oplus I_{n-2}$. Now, $\text{tr}(A) = 0$ (110) but $\text{tr}(PAP^{-1}) = j$.

Theorem 14 Let $A \in M_n(\mathbb{H})$. Then A is a real scalar matrix if and only if $\text{tr}(A) = \text{tr}(PAP^{-1})$ for all nonsingular matrix $P \in M_n(\mathbb{H})$.

Proof. If A is a real scalar matrix, then $AB = BA$ for every $b \in M_n(\mathbb{H})$. Thus $\text{tr}(PAP^{-1}) = \text{tr}(PP^{-1}A) = \text{tr}A$. Conversely, suppose that $\text{tr}(A) = \text{tr}(PAP^{-1})$ for all nonsingular matrix $P \in M_n(\mathbb{H})$. By Theorem 13, A is Hermitian. Suppose A is not a diagonal matrix. Let the (s, t) entry of A be nonzero for $s \neq t$ and write that nonzero entry as $a+bi+cj+dk$. Since A is Hermitian, the (t, s) entry of A is $a-bi-cj-dk$. Take a permutation matrix T such that $TAT^{-1} = TAT^*$ has its $(1, 2)$ entry equal to $a+bi+cj+dk$. Since TAT^* is also Hermitian, its $(2, 1)$ entry is $a-bi-cj-dk$ and its first and second diagonal entries are real, which we denote as e and f , respectively. Let $S = \begin{bmatrix} 1 & j \\ -j & 2 \end{bmatrix} \oplus I_{n-2}$. One computes that the 2-by-2 leading principal submatrix of $STA(ST)^{-1}$ is

$$\begin{bmatrix} 3aj + 3bk + c - 3di + 2e - f & 2a + 2bi + 2dk - ej + fj \\ 5a - 5bi - 3cj - 5dk - 2ej + 2fj & -3aj + 3bk - c - 3di - e + 2f \end{bmatrix} \quad (3)$$

and that the other diagonal entries of TAT^* are unchanged. If $STA(ST)^{-1}$ is not Hermitian, then, by Theorem 13, there exists $U \in \mathbf{U}_n$ such that $\text{tr}(USTA(UST)^{-1}) \neq \text{tr}(STA(ST)^{-1}) = \text{tr}(A)$, which is a contradiction. Hence $STA(ST)^{-1}$ is Hermitian. From the 2-by-2 leading principal submatrix of $STA(ST)^{-1}$, we see that $\overline{2a + 2bi} + 2dk - ej + \overline{ff} = 5a - 5bi - 3cj - 5dk - 2ej + 2ff$ and so $a=b=d=0$. To conclude that $c = 0$, we take $R = \begin{bmatrix} 1 & i \\ -i & 2 \end{bmatrix} \oplus I_{n-2}$ and use similar arguments on $RTA(RT)^{-1}$. This is a contradiction since $a+bi+cj+dk$ is nonzero. Hence A is a diagonal matrix. To show that A is a scalar matrix, we suppose without loss of generality that its 2-by-2 leading principal submatrix is $\text{diag}(e, f)$ where e and f are real and distinct. Let $S = \begin{bmatrix} 1 & i \\ -i & 2 \end{bmatrix} \oplus I_{n-2}$. Then SAS^{-1} has its 2-by-2 leading principal submatrix equal to $\begin{bmatrix} 2e-f & i(f-e) \\ 2i(f-e) & -e+2f \end{bmatrix}$. If SAS^{-1} is not Hermitian, there exists unitary U such that $\text{tr}(USA(US)^{-1}) \neq \text{tr}(SAS^{-1})$, which is a contradiction. Hence, SAS^{-1} is Hermitian, and so $\begin{bmatrix} 2e-f & i(f-e) \\ 2i(f-e) & -e+2f \end{bmatrix}$ is Hermitian. Thus $\overline{i(f-e)} = 2i(f-e)$, which is a contradiction. Thus, all the diagonal entries of A are real and equal, that is, A is a real scalar matrix.

Corollary 15. Let $A \in M_n(\mathbf{H})$. Then $AB = BA$ (127) for every $b \in M_n(\mathbf{H})$ if and only if $A = rI$ (127) where $r \in \mathbf{R}$.

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