UNITARY AND ORTHOGONAL EQUIVALENCE OF SETS OF MATRICES

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Abstract. Two matrices $A$ and $B$ are called unitary (resp. orthogonal) equivalent if $AU = VB$ for two unitary (resp. orthogonal) matrices $U$ and $V$. Using trace identities, criteria are given for simultaneous unitary, orthogonal or complex orthogonal equivalence between two sets of matrices.

1. Introduction

Let $\{A_1, A_2, \cdots, A_k\}$ and $\{B_1, B_2, \cdots, B_k\}$ be two sets of complex matrices of size $m \times n$. We say that $\{A_i\}$ and $\{B_i\}$ are (simultaneous) unitary equivalent if there exist two unitary matrices $U, V$ of respective dimension such that

$$V^*A_iU = B_i, \quad i = 1, \cdots, k,$$

where $*$ means the transpose and conjugation. Two sets of real (resp. complex) matrices $\{A_i\}, \{B_i\}$ of the same size are said to be orthogonal (resp. complex orthogonal) equivalent if there are orthogonal (resp. complex orthogonal) matrices $P$ and $Q$ such that $Q^tA_iP = B_i$ for all $i$. When the matrices are square matrices and $U = V$, then two sets are said to be (simultaneous) unitary similar. We also say that $\{A_i\}$ are simultaneous complex orthogonal similar to $\{B_i\}$ if $A_iO = OB_i$ for a complex matrix $O$ such that $OO^t = O^tO = I$.

Simultaneous unitary similarity has been an important problem in representation theory. When the set of matrices has no group structure, one of the first nontrivial results was given by Specht [12], and the question has been studied by many people, see in particular [4] for its history and difficulty. In [7] algorithms are given to related problems on simultaneous unitary similarity or congruence for complex square matrices (see also [2]). Recently, important applications are found in quantum computation, where a key question of local unitary equivalence between two quantum states has been reduced to simultaneous orthogonal equivalence between two sets of real matrices (cf. [9]). Current resurgent interest in quiver theory is also a reflection of the importance of the problem.

Geometrically (1.1) represents the matrix representation of a set of linear transformations under common change of orthonormal bases in the domain and range spaces.

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If we relax (1.1) to only require that $A_ip = QB_i$ for two non-singular matrices $P, Q$ of respective dimensions, then $A_i$ and $B_i$ are two matrix representations of a set of linear transformations $L_i$ under different bases. The special case of two linear transformations ($k = 2$) was answered by Kronecker’s theory [6] of the matrix pencil $A_1 + \lambda A_2$ using elementary divisors. In further special cases of symmetric and antisymmetric matrices there are canonical forms under similarity [13]. But for the corresponding unitary problem appropriate verifiable conditions of $P$ and $Q$ are needed. In various applications in quantum computation, one is concerned with the problem of how to judge simultaneous orthogonal equivalence rather than finding the intertwining matrix, as the final solution relies on the relevant problem in invariant theory.

In this note we will give criteria for (1.1) and its analogues and show that two sets of complex (real/complex) matrices are unitary (orthogonal/complex orthogonal) equivalent if and only if the corresponding traces of words in $A_iA_j^*$ (resp. $A_iA_j^t$) are invariant. Usually the real version of a problem is harder, fortunately there is a satisfactory solution for almost all of our statements thanks to a simple argument to pass from the complex numbers to the real numbers. Our approach uses some results from semigroup theory. As an application, we also obtain an alternative version of Albert’s criterion for simultaneous similarity of symmetric matrices (Remark 2.6), which avoids the complicated special cases in the original argument.

We remark that a care is made to be self-contained and to indicate the generalization to semigroups from the corresponding results in finite groups.

2. Square matrices

We first consider the unitary similarity (resp. orthogonal similarity) of two sets of complex (resp. real) square matrices. Let $\{A_i\}$ be a set of complex (resp. real) matrices of same dimension. We say that $\{A_i\}$ is hermitian closed (resp. transpose closed) if each $A_i^*$ (resp. $A_i^t$) is contained in the span $\langle A_i \rangle$ of the set $\{A_i\}$. Two sets $\{A_i\}$ and $\{B_i\}$ of complex (resp. real) square matrices of equal dimension are said to be unitary similar (resp. orthogonal similar) if there exists a unitary (resp. orthogonal) matrix $U$ such that $U^*A_iU = B_i$ for all $i$, or equivalently $U$ intertwines $A_i$ and $B_i$ for all $i$.

Let $S$ be a set of matrices of equal dimension, a (product) word $w(S)$ in the alphabet $S$ is a matrix product $xy \cdots z$, where $x, y, \ldots, z$ are arbitrary matrices in $S$. We use $W(S) = \{w(S)\}$ to denote the set of words in the alphabet $S$.

To give our first main result we need to recall some basic notions of semigroups and their modules. A set $G$ is a semigroup if there is a closed binary operation on $G$ that satisfies associativity and has an identity. If every element of $G$ is invertible, then $G$ becomes a group. We follow [8, I] to say that a vector space $V$ is a $G$-module if there is an action of $G$ on $V$: $G \times V \ni (x, v) \mapsto x.v \in V$ such that $x.(y.v) = (xy).v$ for all $x, y \in G, v \in V$. We assume that all modules considered in this paper are finite dimensional left modules, but we do not assume that the semigroup $G$ is finite. Equivalently if $G$ is a (semi)group of linear transformations on $V$, then $V$ is a $G$-module.
with the action given by the transformation. In this case, the entries of the matrix representation are called the \textit{coordinate functions} of \( G \).

Two \( G \)-modules \( V_i \) are called \textit{equivalent} or \textit{isomorphic}, denoted by \( V_1 \cong V_2 \), if there is a linear map \( \phi : V_1 \rightarrow V_2 \) such that \( x.\phi(v) = \phi(x.v) \) for all \( x \in G, v \in V \). In terms of the matrix representation, this means that \( xP = Px \) (\( \forall x \in G \subset \text{End}(V) \)) for some non-singular matrix \( P \).

The notions of \textit{reducible}, \textit{completely reducible} and \textit{decomposable} \( G \)-modules can be defined as in the situation of group modules (cf. \cite{I}). The most useful ones for us are (i) \( V \) is an irreducible \( G \)-module if \( V \) has no non-trivial \( G \)-submodules. It is known that the Schur lemma holds in this case, i.e., the only \( G \)-homomorphism between two irreducible \( G \)-modules are scalar homomorphisms. (ii) \( V \) is a completely reducible \( G \)-module if \( V \cong V_1 \oplus \cdots \oplus V_r \) where \( V_i \) are irreducible.

If \( G \) is a semigroup of linear transformations on \( V \), then the associated \( G \)-module \( V \) is reducible iff under the matrix representation, every element of \( G \) is uniformly of the block triangular form \( x = \begin{bmatrix} x_1 & 0 \\ x_3 & x_2 \end{bmatrix} \) of fixed shape, where \( x_1 \) and \( x_3 \) are square matrices of size smaller than that of \( x \); and \( V \) is \textit{decomposable} if all \( x = \begin{bmatrix} x_1 & 0 \\ 0 & x_2 \end{bmatrix} \) with the fixed shape.

A \( G \)-module \( V \) is called \textit{unitary} if there exists a positive-definite hermitian form \((,\) on \( V \) such that \((xu, xv) = (u, v) \) for any \( x \in G \), and arbitrary \( u, v \in V \). Equivalently the corresponding linear transformations of the elements of \( G \) are represented by unitary matrices. In the case of a transpose-closed \( G \)-module, this is equivalent to the existence of a \( G \)-invariant symmetric bilinear form on \( V \).

The \textit{character} \( \chi(V) \) of \( G \)-module \( V \) is the trace function \( \chi(V)(x) = \text{tr}_V(x), x \in G \). We will show that two irreducible \( G \)-modules are equivalent iff their characters are the same (Theorem 2.1).

In finite group theory, every complex module is completely reducible (Maschke’s theorem). For the semigroup theory, this is not true in general, but we still have some form of Maschke’s theorem for (possibly infinite) semigroups.

The following theorem was mainly due to Frobenius and Schur \cite{S} for linear transformations. We remark that the statements hold for semigroups of transpose closed linear transformations as well.

\textbf{Theorem 2.1.} Let \( G \) be a semigroup. (1) If \( V \) is a unitary \( G \)-module, then \( V \) is completely reducible. (2) Two completely reducible \( G \)-modules are equivalent if and only if their characters are equal.

\textit{Proof.} (i) The idea of the proof is to show that if \( V \) is unitary reducible, then it is also unitary decomposable, i.e. the submodule has a complementary submodule or it is a direct summand. Using the matrix representation, this boils down to the fact that a block triangular matrix must be block diagonal if it is invariant under \(*\)-operation.
(ii) Since completely reducible modules are direct sums of irreducible modules, by adding necessary irreducible summands with possibly zero multiplicity, we can write the completely reducible modules as
\[ V = V_1^{a_1} \oplus \cdots \oplus V_r^{a_r}, \quad a_i \in \mathbb{Z}_+ \]
\[ U = V_1^{b_1} \oplus \cdots \oplus V_r^{b_r}, \quad b_i \in \mathbb{Z}_+ \]
where \( V_i \) are pairwise inequivalent irreducible \( G \)-modules and assume that \( \chi(V) = \chi(U) \). Taking characters we have
\[ (a_1 - b_1)\chi(V_1) + \cdots + (a_r - b_r)\chi(V_r) = 0. \]
By a theorem of Frobenius and Schur [5] (cf. [3, Th. 27.8]) the coordinate functions of pairwise inequivalent irreducible modules for semigroups are linearly independent, their characters are thus linearly independent. Therefore \( a_i = b_i \) for \( i = 1, \ldots, r \), i.e. \( V \simeq U \).

We now come to our first result. It was announced in [11]. The special case of a pair of matrices is the Specht criterion [12] for \( \{A, A^*\} \) and \( \{B, B^*\} \). Since the basic results and notions for semigroups are prepared above, a simple proof can be furnished as follows.

**Theorem 2.2.** Let \( \{A_i\} \) and \( \{B_i\} \) be two sets of \( n \times n \) hermitian closed complex matrices. Then \( \{A_i\} \) and \( \{B_i\} \) are unitary similar if and only if \( \text{tr}(w\{A_i\}) = \text{tr}(w\{B_i\}) \) for any word \( w \).

**Proof.** Let the index set of \( \{A_i\} \) be \( I \), and consider the free semigroup \( G \) generated by \( y_1, \ldots, y_{|I|} \). The assignment \( y_i \mapsto A_i \) (resp. \( B_i \)) defines a representation \( V_A \) (resp. \( V_B \)) of \( G \) on the \( n \)-dimensional space \( V = \mathbb{C}^n \). Their associated \( G \)-modules are also denoted by \( V_A \) and \( V_B \) as well.

The hermitian closedness implies that both modules \( V_A \) and \( V_B \) are unitary completely reducible modules for the free semigroup \( G \). Since the trace of every word in \( G \) are the same, \( V_A \) and \( V_B \) have the same character \( \chi(V_A) = \chi(V_B) \). By Theorem 2.1 it follows that \( V_A \simeq V_B \), so there exists a non-singular matrix \( P \) such that
\[ A_i P = P B_i, \quad i = 1, \ldots, k. \]
Since \( \{A_i\} \) and \( \{B_i\} \) are hermitian closed, we also have
\[ P^* A_i = B_i P^*, \quad i = 1, \ldots, k. \]
Then \( PP^* A_i = PB_iP^* = A_i PP^* \). As \( PP^* \) is positive semi-definite, we let \( (PP^*)^{1/2} \) be the square root of \( PP^* \). Then \( (PP^*)^{1/2} \) also commutes with \( A_i \) for all \( i \). Let \( U \) be the unitary part of \( P \) in the polar decomposition. Subsequently \( U = (PP^*)^{-1/2} P \) intertwines with \( A_i \) and \( B_i \) for all \( i \), i.e. \( A_i U = UB_i \) for \( i \).

It can be shown that only finitely many trace identities are needed. For a pair of matrices, the bound of the word length is \( n \sqrt{\frac{2n^2}{4(n-1)} + \frac{1}{4} + \frac{n^2}{2}} \) [10]. For sets of real
symmetric matrices under Jordan-closeness, the bound can be improved (see Remark 2.6). The real version of the theorem also holds.

**Corollary 2.3.** Let \( \{A_i\} \) and \( \{B_i\} \) be two sets of real square matrices of the same size and assume that both sets are closed under transpose. Then \( \{A_i\} \) and \( \{B_i\} \) are orthogonal similar iff \( \text{tr}(w(A_i)) = \text{tr}(w(B_i)) \) for any word \( w \) in respective alphabets, and iff there is a real matrix \( P \) such that \( PA_iP^{-1} = B_i \) for all \( i \).

**Proof.** By Theorem 2.2, the trace identity implies there exists a unitary matrix \( U \) such that \( A_iU = UB_i \) for any \( i \). Let \( P \) and \( Q \) be the real and imaginary part of \( U \), then one of them is nonsingular, say \( P \). Taking the real part of the intertwining equation, we obtain that \( A_iP = PB_i \) for any \( i \). Let \( O \) be the orthogonal part of \( PP^t \) in its polar decomposition, then the same argument of Theorem 2.2 gives that \( A_iO = OB_i \) for all \( i \). \( \square \)

If we replace the hermitian closeness condition by transpose closeness, then we have the following result.

**Theorem 2.4.** Let \( \{A_i\} \) and \( \{B_i\} \) be two sets of \( n \times n \) transpose closed complex matrices. Then \( \{A_i\} \) and \( \{B_i\} \) are complex orthogonal similar if and only if \( \text{tr}(w(\{A_i\})) = \text{tr}(w(\{B_i\})) \) for any word \( w \) in respective alphabets.

**Proof.** We noted that Theorem 2.2 holds for semigroups of matrices that are transpose closed. The same proof of Corollary 2.3 can be repeated to derive the result. \( \square \)

**Remark 2.5.** The criteria do not hold without the condition of hermitian or transpose closeness. For example let \( A = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \). Then \( \text{tr}(A^n) = \text{tr}(B^n) \), but \( A \) is not similar to \( B \).

The following application modifies Albert’s criterion on simultaneous similarity of real symmetric matrices.

**Remark 2.6.** Let \( \{A_i\} \) and \( \{B_i\} \) be two sets of \( k \) real symmetric matrices. Suppose that the traces of any corresponding words in \( A_i \) and \( B_i \) are identical. By a classical fact that any symmetric polynomial is a polynomial in the power-sum symmetric polynomials, it follows that \( \det(xI - A) = \det(xI - B) \) for any linear combination \( A = \sum_{i=1}^{k} x_iA_i \) and \( B = \sum_{i=1}^{k} x_iA_i \), where \( x, x_i \) are indeterminates. Albert’s criterion \cite{Albert} says that \( \{A_i\} \) is “almost” simultaneous orthogonal similar to \( \{B_i\} \) if the determinant identity holds plus that \( \{A_i\} \) and \( \{B_i\} \) are Jordan-closed, i.e. closed under anti-commutators \( \{X,Y\} = XY + YX \) for any members of the sets. Here “almost” means that there are some counterexamples of degree 2 simple Jordan algebras of dimension \( 4q_i + 2 \). Moreover, \cite{Albert} showed that these “counterexamples” can be removed if certain monomials in \( \{A_i\} \) and \( \{B_i\} \) of length \( 4q_i + 2 \) have the same traces. In particular, one only needs to verify the trace identity for word length \( \leq \max(n, 4q_i + 2) \) to ensure the simultaneous similarity of \( \{A_i\} \) to \( \{B_i\} \) under the condition of Jordan-closeness.
3. Rectangular matrices

The following elementary fact is needed for further discussion.

**Lemma 3.1.** Let $a, b \in \mathbb{C}^n$ (resp. $\mathbb{R}^n$) be two column vectors. Then $aa^* = bb^*$ iff there is a complex number $\theta$, $|\theta| = 1$ (resp. $\theta = \pm 1$) such that $a = \theta b$.

**Proof.** Let $a = (a_1, \ldots, a_n)^t$ and $b = (b_1, \ldots, b_n)^t$. Clearly $a_i = 0$ iff $b_i = 0$, so we can assume that $a_1, \ldots, a_k$ are non-zero numbers, and $a_{k+1} = \cdots = a_n = 0$. Since $|a_i|^2 = |b_i|^2 \neq 0$, we can write $a_i = \theta_i b_i$ with $|\theta_i| = 1$ for each $i = 1, \ldots, k$. But $a_i \bar{a}_j = b_i \bar{b}_j \neq 0$ imply that $\theta_i \bar{\theta}_j = 1$ for any $i, j = 1, \cdots, k$. Therefore $\theta_1 = \cdots = \theta_k = \theta$. Then we have that $a = \theta b$. □

We have the following generalization.

**Lemma 3.2.** Let $A, B$ be two $m \times n$-matrices over $\mathbb{C}$ (resp. $\mathbb{R}$). Then $AA^* = BB^*$ iff there is a unitary (resp. orthogonal) matrix $V$ such that $A = BV$.

**Proof.** The sufficient direction is clear. On the other hand, let $U = [u_1, \ldots, u_m]$ be the unitary matrix of a basis of orthonormal eigenvectors of $AA^* = BB^*$. Suppose the first $r$ eigenvectors have nonzero eigenvalues $\sigma_i^2$, then $v_i = \sigma_i^{-1} A^* u_i$ exhaust all eigenvectors of $A^* A$ with non-zero eigenvalues (same eigenvalue $\sigma_i^2$). Extend $\{v_1, \ldots, v_r\}$ into a unitary matrix $V_1 = [v_1, \ldots, v_n]$ of a basis of orthonormal eigenvectors for $A^* A$. Then $AV_1 = UD, A^* U = V_1 D^t$, where $D = \begin{pmatrix} D_1 & 0 \\ 0 & 0 \end{pmatrix}_{m \times n}$ and $D_1 = \text{diag}(\sigma_1, \ldots, \sigma_r)$. Similarly there exists another unitary matrix $V_2$ such that $BV_2 = UD, B^* U = V_2 D^t$. Subsequently $A = BV_2 V_1^{-1}$. □

**Theorem 3.3.** Let $\{A_i\}$ and $\{B_i\}$ be two sets of complex (resp. real) $m \times n$-matrices. The following are equivalent.

(a) the set $\{A_i\}$ is unitary equivalent (resp. orthogonal equivalent) to the set $\{B_i\}$;

(b) the set $\{A_i A_j^*|i \leq j\}$ is unitary similar (resp. orthogonal similar) to the set $\{B_i B_j^*|i \leq j\}$;

(c) $\text{tr } w(\{A_i A_j^*\}) = \text{tr } w(\{B_i B_j^*\})$ for any word $w$ in respective alphabets.

**Proof.** Equivalence of (b) and (c). Suppose (b) holds, then there is a unitary matrix $U$ such that $U^* A_i A_j^* U = B_i B_j^*$ for any $i \leq j$. Taking * we also have $U^* A_j A_i^* U = B_j B_i^*$ for any $i \leq j$, then $U^* A_i A_j^* U = B_i B_j^*$ hold for any $i, j$. Therefore the set $\{A_i A_j^*|i, j\}$ is simultaneous unitary equivalent to the set $\{B_i B_j^*|i, j\}$, so (c) holds by Theorem 2.2.

The converse direction is guaranteed by Theorem 2.2.

(b) clearly follows from (a). We now show that (b) implies (a). Let $A$ be the block matrix defined by $A^* = [A_i^*, \ldots, A_k^*]$. Then the block matrix $AA^* = [A_i A_j^*]$ with $(i, j)$-entry being an $m \times m$ matrix $A_i A_j^*$. By the argument above (b) implies that there is a unitary matrix $U$ such that

$$UA_i A_j^* U^* = B_i B_j^*$$

for any $i \leq j$. □
for any $i, j$. Then
\[
\begin{pmatrix}
UA_1 \\
\vdots \\
UA_k
\end{pmatrix}
\begin{bmatrix}
A_1^* & \cdots & A_k^*
\end{bmatrix}
= 
\begin{pmatrix}
B_1 \\
\vdots \\
B_k
\end{pmatrix}
\]
\[(3.4)
\]
Using Lemma 3.2 for the block matrices
\[
\begin{pmatrix}
UA_1 \\
\vdots \\
UA_k
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
B_1 \\
\vdots \\
B_k
\end{pmatrix},
\]
we get a unitary $m \times m$-matrix $V$ such that
\[
\begin{pmatrix}
UA_1 \\
\vdots \\
UA_k
\end{pmatrix}
= 
\begin{pmatrix}
B_1 \\
\vdots \\
B_k
\end{pmatrix}
V.
\]
Subsequently $UA_i = B_i V$ for all $i$.

The real case follows by a similar argument in view of Corollary 2.3. $\square$

The following result is clear from our discussion.

**Theorem 3.4.** Let $\{A_i\}$ and $\{B_i\}$ be two sets of complex $m \times n$-matrices. The following are equivalent.

(a) the set $\{A_i\}$ is complex orthogonal equivalent to $\{B_i\}$;

(b) the set $\{A_i A_j^* | i \leq j\}$ is complex orthogonal similar to $\{B_i B_j^* | i \leq j\}$;

(c) $\text{tr } w(\{A_i A_j^*\}) = \text{tr } w(\{B_i B_j^*\})$ for any word $w$ in respective alphabets.

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