THE CORRELATION NUMERICAL RANGE AND
TRACE–POSITIVE COMPLEX POLYNOMIALS

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Abstract. Let $A \in M_n(\mathbb{C})$. We prove that if $W_c(A)$, the correlation numerical range introduced in [2], is a subset of $[0, \infty)$, then $A = P + D$ where P is positive semidefinite and D is a diagonal matrix such that $Tr(D) = 0$. This answers a question of D. Hadwin and D. Han. Additionally, we explore a few properties of $W_c(A)$ and $W_{uc}(A)$, another numerical range introduced in [2] that is closely related to Connes's Embedding Conjecture.

1. Introduction

The numerical range $W(A) = \{ \langle A\xi, \xi \rangle : \xi \in \mathbb{C}^n, \|\xi\| = 1 \}$ of a matrix $A \in M_n(\mathbb{C})$ is the collection of images of A under all vector states of $M_n(\mathbb{C})$ in its usual representation on $\mathbb{C}^n$. Since any irreducible representation of $M_n(\mathbb{C})$ is unitarily equivalent to this usual representation, every pure state of $M_n(\mathbb{C})$ is a vector state. This, the Krein-Milman Theorem, and the fact (the Toeplitz-Hausdorff Theorem) that $W(A)$ is compact and convex, yields the alternative expression

$$W(A) = \{ \tau_n(AB) : B \in M_n^+(\mathbb{C}), \, \tau_n(B) = 1 \},$$

where $\tau_n = \frac{1}{n} Tr$ denotes the normalized trace on $M_n(\mathbb{C})$. Replacing positive semidefinite matrices of unit trace by the subset of such matrices with ones along the diagonal (i.e. correlation matrices), we obtain the *correlation numerical range* defined and studied in [2]:

$$W_c(A) = \{ \tau_n(AB) : B \in M_n^+(\mathbb{C}), \, diag(B) = I_n \}.$$

It is a well–known basic fact that $W(A) \subseteq \mathbb{R}$ if and only if A is self–adjoint, and that $W(A) \subseteq [0, \infty)$ if and only if A is positive semidefinite. In contrast, $W_c(A) \subseteq \mathbb{R}$ if and only if A is the sum of a self–adjoint matrix and a diagonal matrix with zero trace (cf. Theorem 1 of [2]), and if A is the sum of a positive semidefinite matrix and a trace–zero diagonal matrix, then $W_c(A) \subseteq [0, \infty)$. The question of whether the converse statement is true appears as Problem 1 of [2]:

PROBLEM 1.1. *If $A \in M_n(\mathbb{C})$ and $W_c(A) \subseteq [0, \infty)$, must there exist positive semidefinite P and trace–zero diagonal D in $M_n(\mathbb{C})$ such that $A = P + D$?*

In the present paper we solve the above problem in the affirmative. In [2] it is shown that Problem 1.1 is related to the famous Connes Embedding Conjecture in the following way. The numerical range obtained by considering only *unitarily induced correlation matrices*

$$W_{uc}(A) = \{\tau_n(AB) : \exists m \in \mathbb{N}, \exists \{U_k\}_{k=1}^n \subseteq \mathscr{U}(M_m(\mathbb{C})) \text{ s.t. } \forall i, j, \ B_{ij} = \tau_m(U_j^* U_i)\}$$

leads to the following, which has an affirmative answer if and only if the Connes Embedding Conjecture also does:

CONJECTURE 1.2. *Let $A = (A_{ij})_{i,j=1}^n \in M_n(\mathbb{C})$, let $u_1, ..., u_n$ be the generators of the free group $\mathbb{F}_n$, and let $p_A(u_1, ..., u_n) = \sum_{i,j=1}^n A_{ij} u_i^* u_j \in \mathbb{C}\mathbb{F}_n$. If $W_{uc}(A) \subseteq (0, \infty)$ then there exists $m \in \mathbb{N}$ such that there are q_i, f_i and g_i in $\mathbb{C}\mathbb{F}_n$ for all $i \in \{1, 2, ..., m\}$, satisfying*

$$p_A(u_1, ..., u_n) = \sum_{i=1}^m q_i^* q_i + \sum_{i=1}^m (f_i g_i - g_i f_i).$$

Furthermore, it is established that, if $A = P + D$ with P positive semidefinite and D trace–zero diagonal, then $p_A(u_1, ..., u_n)$ can be written in the form appearing in the conclusion above. Thus, our affirmative answer to Problem 1.1 implies an affirmative answer to the weak analogue of the Connes Embedding Problem appearing as Problem 3 of [2]. Furthermore, together with the fact that when $A \in M_3(\mathbb{C})$ the two sets $W_c(A)$ and $W_{uc}(A)$ are equal (cf. Lemma 7 of [2]), the affirmative answer to Problem 1.1 for $A \in M_3(\mathbb{C})$ implies an affirmative answer to Conjecture 1.2 in the $n = 3$ case, a result first obtained by Popovych using Tarski's Decidability Theorem [3].

2. Main result

It suffices to solve Problem 1.1 for self–adjoint $A \in M_n(\mathbb{C})$ with constant diagonal (meaning for those for which there exists $c \in \mathbb{R}$ such that $A_{ii} = c$ for all $i \in \{1, ..., n\}$), by Theorem 1 of [2]. Let $\mathscr{D}_{n,0}$ denote the set of all trace-zero diagonal matrices in $M_n(\mathbb{C})$. Throughout, we view $M_n(\mathbb{C})$ as a Hilbert space with inner product $\langle X, Y \rangle = Tr(Y^* X)$, and associated norm denoted by $\|\cdot\|_F$. By Lemma 2 of [2], the convex cone

$$\mathscr{B} = \{B : B = P + D, \ P \geqslant 0 \text{ and } D \in \mathscr{D}_{n,0}\}$$

of $M_n(\mathbb{C})$ is closed.

LEMMA 2.1. *Let $A \in M_n(\mathbb{C})$ be self–adjoint with constant diagonal. Then the $B \in \mathscr{B}$ for which $\|A - B\|_F$ is minimum has constant diagonal.*

Proof. Let $a > 0$ and $i, j \in \{1, 2, ...n\}$, and let $E = E(a, i, j) = a(E_{ii} - E_{jj})$ where E_{kk} denotes the standard $n \times n$ matrix unit with kth diagonal entry 1 and zeros elsewhere. If B is the element of $\mathscr{B}$ such that $\|A - B\|_F$ is minimum, then for any $a > 0$

$$\|A - B\|_F^2 \leqslant \|(A - B) - E)\|_F^2.$$

Expanding the right hand side of the above inequality, we see that

$$\|A - B\|_F^2 \leqslant \|A - B\|_F^2 - 2\langle A - B, E \rangle + \|E\|_F^2,$$

and thus

$$2a(B_{jj} - B_{ii}) = 2\langle A - B, E \rangle \leqslant 4a^2,$$

which implies that

$$B_{jj} \leqslant B_{ii}.$$

Replacing $E(a, i, j)$ with $E(a, j, i)$ in the above yields the reverse inequality, and consequently $B_{jj} = B_{ii}$ for all i, j. $\square$

The following lemma is a well-known and standard result, but is included for the reader's convenience.

LEMMA 2.2. *Let $A \in M_n(\mathbb{C})$ be self–adjoint with constant diagonal. If $\mathscr{B}$ is a closed convex cone in $M_n(\mathbb{C})$ and $B \in \mathscr{B}$ for which $\|A - B\|_F$ is minimum, then $\langle A - B, Q \rangle \leqslant 0$ for every $Q \in \mathscr{B}$, and $\langle B, B - A \rangle = 0$.*

Proof. If $A \in \mathscr{B}$, then $A = B$ and the claim follows immediately. Suppose now that $A \notin \mathscr{B}$. Suppose that $Q \in \mathscr{B}$ with $\|Q\|_F = 1$. For any $t > 0$,

$$\|A - B\|_F^2 \leqslant \langle A - B - tQ, A - B - tQ \rangle$$
$$= \|A - B\|_F^2 - 2t\langle A - B, Q \rangle + t^2,$$

which is true if and only if

$$0 \leqslant -2t\langle A - B, Q \rangle + t^2.$$

Dividing by t and rearranging the inequality establishes that

$$\langle A - B, Q \rangle \leqslant t.$$

Since this holds for all $t > 0$, we have established the first claim that $\langle A - B, Q \rangle \leqslant 0$ for every $Q \in \mathscr{B}$.

Let $Q \in \mathscr{B}$ be arbitrary. If $0 < t < 1$, then since $\mathscr{B}$ is convex, $(1 - t)B + tQ \in \mathscr{B}$, and since B is the nearest point in $\mathscr{B}$ to A we have that

$$\|A - B\|_F^2 \leqslant \|A - ((1 - t)B + tQ)\|_F^2$$
$$= \|A - B + t(B - Q)\|_F^2$$
$$= \|A - B\|_F^2 + 2t\langle A - B, B - Q \rangle + t^2 \|B - Q\|_F^2.$$

Subtracting $\|A - B\|_F^2$ from both sides, dividing both sides by t, multiplying by -1 and letting $t \to 0$ we obtain that

$$\langle A - B, Q - B \rangle \leqslant 0$$

for all $Q \in \mathscr{B}$. Particularly, since $\mathscr{B}$ is closed, $0 \in \mathscr{B}$ and so $\langle A - B, -B \rangle \leqslant 0$, which implies $\langle A - B, B \rangle \geqslant 0$. Together with the inequality $\langle A - B, B \rangle \leqslant 0$ obtained above, we have that $\langle A - B, B \rangle = 0$ and the final claim follows.   □

We now prove the main theorem.

THEOREM 2.3. *Let $A \in M_n(\mathbb{C})$ be self–adjoint with constant diagonal such that $Tr(AB) \geqslant 0$ for every correlation matrix $B \in M_n(\mathbb{C})$. Then there exists $P \geqslant 0$ in $M_n(\mathbb{C})$ and $D \in \mathscr{D}_{n,0}$ such that $A = P + D$.*

Proof. Assume that A is self–adjoint with constant diagonal and satisfies $Tr(AC) \geqslant 0$ for all $C \geqslant 0$ with constant diagonal, and that $B \in \mathscr{B}$ for which $\|A - B\|_F$ is a minimum. Then by Lemma 2.1 $A - B$ has constant diagonal and by Lemma 2.2 we have $\langle A - B, Q \rangle \leqslant 0$ for all $Q \geqslant 0$. Therefore, $B - A \geqslant 0$ and has constant diagonal. It follows from the hypothesis that $\langle A, B - A \rangle \geqslant 0$ and from Lemma 2.2 that $\langle B, B - A \rangle = 0$. Therefore $\langle A - B, B - A \rangle \geqslant 0$ and $\|A - B\|_F \leqslant 0$ and hence $A = B$.   □

3. Further properties of W_c and W_{uc}

We now collect a few further results to clarify the relationship between the solution to Problem 1.1 and the Connes Embedding Conjecture. For what follows, recall that any matrix $A \in M_n(\mathbb{C})$ can be conveniently decomposed as $A = \frac{A+A^*}{2} + i\frac{A-A^*}{2i} = Re(A) + iIm(A)$. We first note the following natural abstract characterization of $W_c(\cdot)$, which is analogous to a similar characterization of the classical numerical range $W(\cdot)$.

THEOREM 3.1. *Let $\mathscr{P}(\mathbb{C})$ denote the power set of $\mathbb{C}$. If $f : M_n(\mathbb{C}) \to \mathscr{P}(\mathbb{C})$ such that for every matrix A in $M_n(\mathbb{C})$ the following conditions hold:*
(i) $f(A)$ is a compact, convex set;
(ii) $f(\alpha A + \lambda I_n) = \alpha f(A) + \lambda$ for all $\alpha, \lambda \in \mathbb{C}$;
(iii) $f(A) \subseteq \{t + is : t \geqslant 0, s \in \mathbb{C}\}$ if and only if $Re(A) = P + D$ for some $P \geqslant 0$ and trace-zero diagonal D.
Then $f(A) = W_c(A)$ for all $A \in M_n(\mathbb{C})$. (I.e. $W_c : M_n(\mathbb{C}) \to \mathscr{P}(\mathbb{C})$ is the only function on $M_n(\mathbb{C})$ satisfying the properties (i) through (iii).)

Proof. Let $A \in M_n(\mathbb{C})$, and suppose there exists another function f satisfying the three aforementioned properties. Suppose that $W_c(A) \nsubseteq f(A)$, meaning that there exists a $\lambda \in \mathbb{C}$ such that $\lambda \in W_c(A)$ but $\lambda \notin f(A)$. Because $\{\lambda\}$ and $f(A)$ are both compact and convex sets, then there exists a line in the complex plane separating the two sets; we can rotate this line (and the two sets) so that it coincides with the imaginary axis, which is to say we can select complex numbers $\alpha_1 \neq 0$ and α_2 such that $Re(\alpha_1 \lambda + \alpha_2) < 0$, whereas $\alpha_1 f(A) + \alpha_2$ is contained in the closed right half-plane.

Now, define $\lambda' = \alpha_1\lambda + \alpha_2$ and $A' = \alpha_1 A + \alpha_2 I_n$. Because λ' is contained in $W_c(A')$, it cannot be contained within the closed right half-plane, implying that $Re(A')$ cannot be written as $P + D$, where $P \geqslant 0$ and $D \in \mathscr{D}_n$. However, $\alpha_1 f(A) + \alpha_2 = f(\alpha_1 A + \alpha_2 I_n) := f(A')$ *is* contained within the closed right half-plane, which means that $Re(A')$ *can* be written as $P + D$, which is clearly a contradiction. Therefore, $W_c(A) \subseteq f(A)$ must be true.

Reversing in which set λ is assumed to be will force $f(A) \subseteq W_c(A)$ to be true, and therefore $W_c(A) = f(A)$. $\square$

In what follows, we use UIC to abbreviate "unitarily induced correlation."

THEOREM 3.2. *Let $A \in M_n(\mathbb{C})$. If $W_{uc}(A) \subseteq \mathbb{R}$, then $A = H + D$, where H is self-adjoint and D is trace-zero diagonal.*

Proof. Let $A = Re(A) + iIm(A)$ be some matrix in $M_n(\mathbb{C})$. By the assumption that $\tau_n(AB) \in \mathbb{R}$ for every UIC matrix B, we see that when $B = I_n$ (which we will momentarily show is a UIC matrix) $Im(A)$ is forced to be a trace-zero matrix, which we shall now denote as C.

Now, let $\{U_1, U_2, ..., U_n\}$ be a collection of pairwise orthogonal unitary matrices (i.e., $\langle U_i, U_j \rangle = \tau_n(U_j^* U_i) = 0$ for all $i \neq j$). An example of one such collection can be procured by letting $U_1 = I_n$ and $U_k = V^{k-1}$, for $k \geqslant 2$, where $V = E_{12} + E_{23} + ... + E_{n1}$ is the cyclic unitary permutation of order n. First, note that the correlation matrix associated with such an orthonormal collection is the identity matrix I_n, which therefore makes it a UIC matrix. Now, suppose that $i < j$. Since our purpose is to isolate arbitrary off-diagonal entries, replace U_i with zU_j, where z is some complex number with unit modulus. This modified collection of unitaries will produce the UIC matrix $I_n + zE_{ij} + \overline{z}E_{ji}$. Because $\tau_n(CB) = 0$ is true for every UIC B, we can say that $\tau_n(CB_1) - \tau_n(CB_2) = 0$. Choosing $B_1 = I_n + zE_{ij} + \overline{z}E_{ji}$ and $B_2 = I_n$ gives us $\tau_n(CB_1) - \tau_n(CB_2) = 2Re(z\overline{C}_{ij}) = 0$, which must hold for z with the above mentioned property. Replacing z with iz gives us $Re(z\overline{C}_{ij}) = iIm(z\overline{C}_{ij})$, which implies $z\overline{C}_{ij} = 0$, and therefore $C_{ij} = 0$. Finally, we see that $C = Im(A)$ is a trace-zero diagonal matrix. $\square$

One might optimistically attempt to show that $W_{uc}(A) \subseteq [0, \infty)$ implies that $W_c(A) \subseteq [0, \infty)$ for every $A \in M_n(\mathbb{C})$, hoping the smaller set's structure somehow determines the larger, but this will not hold as we now see.

THEOREM 3.3. *Let $\mathscr{C}$ be the closed convex cone generated by the UIC matrices. (i) There exists a correlation matrix B such that $B \notin \mathscr{C}$ if and only if (ii) there exists a self-adjoint A such that $W_{uc}(A) \subseteq [0, \infty)$ but $W_c(A) \not\subseteq [0, \infty)$.*

Proof. The proof of (ii) $\Longrightarrow$ (i) is trivial, since $W_c(A) \not\subseteq [0, \infty)$ implies there exists a correlation matrix B such that $\tau(AB)$ is negative, whereas $W_{uc}(A) \subseteq [0, \infty)$ implies that $\tau(AB) \geqslant 0$ for every UIC correlation matrix B. Now assume that (i) is true. By the Hahn-Banach Theorem, we can separate $\mathscr{C}$ and $\{B\}$ by a hyperplane. Because

the cone $\mathscr{C}$ contains zero, we may implement the separation by an associated linear functional $\varphi(\cdot) = Tr(A\cdot)$ satisfying $Re(Tr(AB)) < 0$ and $Re(Tr(AB')) \geqslant 0$ for all $B' \in \mathscr{C}$, where A is some matrix. This pair of inequalities imply that $Tr(Im(A)B) = 0$ and $Tr(Im(A)B') = 0$; and because $Re(Tr(Re(A)B)) = Tr(Re(A)B)$, we further get that $Tr(Re(A)B) < 0$ and $Tr(Re(A)B') \geqslant 0$ for all $B' \in \mathscr{C}$, where $Re(A)$ is self-adjoint.

Therefore, the implication (i) $\implies$ (ii) is true. In [1] it is shown that there exists such a B, from which it follows that $W_{uc}(A) \subseteq [0, \infty) \implies W_c(A) \subseteq [0, \infty)$ is *not* true. $\square$

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