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In this paper positivity of polynomials in free noncommuting variables in a dimension-dependent setting is considered. That is, the images of a polynomial under finite-dimensional representations of a fixed dimension are investigated. It is shown that unlike in the dimension-free case, every trace-positive polynomial is (after multiplication with a suitable denominator — a Hermitian square of a central polynomial) a sum of a positive semidefinite polynomial and commutators. Together with our previous results this yields the following Positivstellensatz: every trace-positive polynomial is modulo sums of commutators and polynomial identities a sum of Hermitian squares with weights and denominators. Understanding trace-positive polynomials is one of the approaches to Connes' embedding conjecture.

1. Introduction

Interest in positivity questions involving noncommutative polynomials has been recently revived by Helton's seminal paper [2002], in which he proved that a polynomial is a sum of squares if and only if its values in matrices of any size are positive semidefinite. Considering polynomials with *positive trace*, Klep and Schweighofer [2008, Theorem 1.6] observed that Connes' embedding conjecture [1976, Section V, pp. 105–107] on type II_1 von Neumann algebras is equivalent to a problem of describing polynomials whose values at tuples of self-adjoint $d \times d$ matrices (of norm at most 1) have nonnegative trace for every $d \geq 1$. This result is the motivation for the present work. Here we investigate polynomials whose values at tuples of $d \times d$ matrices have nonnegative trace for a *fixed* $d \geq 1$. We show that such a polynomial is (after multiplication with a Hermitian square of a suitable central polynomial) a sum of commutators and of a polynomial whose values at tuples of $d \times d$ matrices are positive semidefinite. The latter were characterized in [Klep and Unger 2010], leading us to the following Positivstellensatz: *every polynomial with nonnegative trace on $d \times d$ matrices is modulo sums of commutators and*

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polynomial identities for $d \times d$ matrices a sum of Hermitian squares with weights and denominators. See Section 4 for a precise formulation.

The organization of this paper is as follows: Section 2 introduces the main notions and interprets them in full matrix algebras, Section 3 considers these notions for free algebras, while Section 4 presents our main results.

2. Basic notions and a motivating example

Let R be an associative ring with 1 and *involution* $a \mapsto a^*$ (that is, $(a+b)^* = a^* + b^*$, $(ab)^* = b^* a^*$ and $a^{**} = a$ for all $a, b \in R$). We denote by $\operatorname{Sym} R := \{a \in R \mid a = a^*\}$ its set of *symmetric* elements. Elements of the form a^*a and $ab - ba$ ($a, b \in A$) are called *Hermitian squares* and *commutators*, respectively. We introduce an equivalence relation (*cyclic equivalence*) on R by declaring $a \overset{\text{cyc}}{\sim} b$ if and only if $a - b$ is a sum of commutators in R. For notational convenience we write

$$\Sigma^2 R := \left\{ \sum a_i^* a_i \mid a_i \in R \right\} \subseteq \operatorname{Sym} R, \quad \Theta^2 R := \left\{ a \in R \mid \exists b \in \Sigma^2 R : a \overset{\text{cyc}}{\sim} b \right\}$$

for the sets of (finite) sums of Hermitian squares, and sums of Hermitian squares and commutators in R, respectively.

Throughout this paper k will denote $\mathbb{R}$ or $\mathbb{C}$.

Matrices. For a concrete example of these notions, consider the ring $R = \mathrm{M}_d(k)$ of real or complex square matrices of a fixed size $d \geq 1$ endowed with the usual (complex conjugate) transposition of matrices, denoted here by $*$. Using $\succeq$ to denote the Löwner partial order (that is, $A \succeq B$ if and only if $A - B$ is positive semidefinite), it is easy to see that for $A \in \mathrm{M}_d(k)$, we have

(A) $A \succeq 0$ if and only if $A \in \Sigma^2 \mathrm{M}_d(k)$;

(B) $\operatorname{tr}(A) = 0$ if and only if $A \overset{\text{cyc}}{\sim} 0$ in $\mathrm{M}_d(k)$;

(C) $\operatorname{tr}(A) \geq 0$ if and only if $A \in \Theta^2 \mathrm{M}_d(k)$.

Let us determine multiplication by which matrices respect these properties.

Lemma 2.1. *Suppose $A \in \mathrm{M}_d(k)$ is such that for all $B \in \mathrm{M}_d(k)$,*

$$B \succeq 0 \quad \Rightarrow \quad AB \succeq 0. \tag{1}$$

Then $A = \lambda$ for some $\lambda \in \mathbb{R}_{\geq 0}$.

Proof. Using (1) with $B = 1$, we obtain $A \succeq 0$. In particular, $A = A^*$. Again by (1), A commutes with all positive semidefinite matrices, hence with all symmetric matrices, which are differences of two positive semidefinite matrices by

$$B = \tfrac{1}{4}(B+1)^2 - \tfrac{1}{4}(B-1)^2.$$

So A is scalar and the desired conclusion follows. $\square$

Lemma 2.2. *Suppose $A \in \mathrm{M}_d(k)$ is such that for all $B \in \mathrm{M}_d(k)$,*

$$\mathrm{tr}(B) = 0 \quad \Rightarrow \quad \mathrm{tr}(AB) = 0. \tag{2}$$

Then $A = \lambda$ for some $\lambda \in k$.

Proof. Write $A = [a_{ij}]_{i,j=1}^{d}$. Let $i \neq j$. Then $B = \lambda E_{ij}$ has zero trace for every $\lambda \in k$. (Here E_{ij} denotes the $d \times d$ *matrix unit* with a one in position (i, j) and zeros elsewhere.) By (2), this implies that $\lambda a_{ij} = \mathrm{tr}(AB) = 0$. Since $\lambda \in k$ was arbitrary, $a_{ij} = 0$.

Now let $B = \lambda(E_{ii} - E_{jj})$. Clearly, $\mathrm{tr}(B) = 0$ and hence

$$\lambda(a_{ii} - a_{jj}) = \mathrm{tr}(AB) = 0.$$

As before, this gives $a_{ii} = a_{jj}$. □

Lemma 2.3. *Suppose $A \in \mathrm{M}_d(k)$ is such that for all $B \in \mathrm{M}_d(k)$,*

$$\mathrm{tr}(B) \geq 0 \quad \Rightarrow \quad \mathrm{tr}(AB) \geq 0. \tag{3}$$

Then $A = \lambda$ for some $\lambda \in \mathbb{R}_{\geq 0}$.

Proof. By Lemma 2.2, A is scalar. In addition to that, $a_{ii} = \mathrm{tr}(AE_{ii}) \geq 0$ by (3), showing that A must be a nonnegative multiple of the identity. □

Likewise we can characterize matrices that map positive semidefinite matrices into matrices with nonnegative trace:

Lemma 2.4. *Suppose $A \in \mathrm{M}_d(k)$ is such that for all $B \in \mathrm{M}_d(k)$,*

$$B \succeq 0 \quad \Rightarrow \quad \mathrm{tr}(AB) \geq 0. \tag{4}$$

In the case $k = \mathbb{R}$, assume moreover that $A = A^*$. Then $A \succeq 0$.

Proof. This is just a restatement of the well-known self-duality of the cone of all positive semidefinite matrices. For $v \in k^d$, let $B = vv^* \succeq 0$. Then

$$0 \leq \mathrm{tr}(AB) = \mathrm{tr}(Avv^*) = \mathrm{tr}(v^*Av) = \langle Av, v\rangle,$$

showing A is positive semidefinite. □

Converses of Lemmas 2.1–2.4 hold as well.

3. Positivity in free algebras

Words and polynomials. Fix $n \in \mathbb{N}$. Let

$$\underline{X} := (X_1, \ldots, X_n) \quad \text{and} \quad \underline{X}^* := (X_1^*, \ldots, X_n^*)$$

denote tuples of n distinct variables (or letters). By $\langle \underline{X}, \underline{X}^* \rangle$ we denote the free monoid on $\{\underline{X}, \underline{X}^*\}$ (consisting of *words* in $\underline{X}, \underline{X}^*$) and let $k\langle \underline{X}, \underline{X}^* \rangle$ be the semigroup algebra of $\langle \underline{X}, \underline{X}^* \rangle$ over k (consisting of *polynomials* in noncommuting variables $\underline{X}$ and $\underline{X}^*$ with coefficients in k). We endow $k\langle \underline{X}, \underline{X}^*\rangle$ with the involution $p \mapsto p^*$ mapping $X_j \mapsto X_j^*$ and extending complex conjugation on k. Thus $k\langle \underline{X}, \underline{X}^*\rangle$ is the free $*$-algebra on $\underline{X}$ over k.

Cyclic equivalence. It is well known and easy to see that trace-zero matrices are sums of commutators, that is, cyclically equivalent to 0. Cyclic equivalence can also be easily tested in $k\langle \underline{X}, \underline{X}^*\rangle$:

(a) For $v, w \in \langle \underline{X}, \underline{X}^*\rangle$, we have $v \overset{\text{cyc}}{\sim} w$ if and only if there are $v_1, v_2 \in \langle \underline{X}, \underline{X}^*\rangle$ such that $v = v_1 v_2$ and $w = v_2 v_1$. That is, $v \overset{\text{cyc}}{\sim} w$ if and only if w is a cyclic permutation of v.

(b) Polynomials

$$f = \sum_{w\in\langle \underline{X},\underline{X}^*\rangle} a_w w \quad \text{and} \quad g = \sum_{w\in\langle \underline{X},\underline{X}^*\rangle} b_w w \quad \text{for } a_w, b_w \in k$$

are cyclically equivalent if and only if for each $v \in \langle \underline{X}, \underline{X}^*\rangle$,

$$\sum_{\substack{w\in\langle \underline{X},\underline{X}^*\rangle \\ w \overset{\text{cyc}}{\sim} v}} a_w = \sum_{\substack{w\in\langle \underline{X},\underline{X}^*\rangle \\ w \overset{\text{cyc}}{\sim} v}} b_w. \tag{5}$$

Evaluations and representations. Let $d \in \mathbb{N}$. An n-tuple of matrices $\underline{A} \in (\mathrm{M}_d(k))^n$ gives rise to a *$*$-representation*

$$\mathrm{ev}_{\underline{A}} : k\langle \underline{X}, \underline{X}^*\rangle \to \mathrm{M}_d(k), \quad p \mapsto p(\underline{A}, \underline{A}^*). \tag{6}$$

We are interested in the values of a *fixed* element $f \in k\langle \underline{X}, \underline{X}^*\rangle$ under all these $*$-representations. If the size d of the matrices A_i is free, we talk about *dimension-free* properties; otherwise we call them *dimension-dependent*. We are mostly interested in the latter, but briefly review the former for the sake of completeness.

Dimension-freeness. Free analogs of properties (A) and (B) have been established, while a free version of (C) is closely related to an important open problem on operator algebras due to Connes; see below for further details.

Let $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$.

$(\mathrm{A})^{\mathrm{fr}}$ $f(\underline{A}, \underline{A}^*) \succeq 0$ for all $d \in \mathbb{N}$ and all $\underline{A} \in \mathrm{M}_d(k)^n$ if and only if $f \in \Sigma^2 k\langle \underline{X}, \underline{X}^*\rangle$;

$(\mathrm{B})^{\mathrm{fr}}$ $\operatorname{tr}\big(f(\underline{A}, \underline{A}^*)\big) = 0$ for all $d \in \mathbb{N}$ and all $\underline{A} \in \mathrm{M}_d(k)^n$ if and only if $f \overset{\text{cyc}}{\sim} 0$ in $k\langle \underline{X}, \underline{X}^*\rangle$.

Part $(\mathrm{A})^{\mathrm{fr}}$ is due to Helton [2002] (see also [McCullough 2001; McCullough and Putinar 2005]), and $(\mathrm{B})^{\mathrm{fr}}$ is Theorem 2.1 of [Klep and Schweighofer 2008]. (This reference will henceforth be abbreviated as [KS 2008].) See also [Collins and Dykema 2008, Lemma 2.9] for a proof inspired by free probability. For a recent study of trace-positive polynomials in a dimension-free setting see also [Netzer and Thom 2010].

The obvious extension of (C) fails: there are $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$ with positive trace everywhere, but still not cyclically equivalent to a sum of Hermitian squares. The following is a variant of the noncommutative Motzkin polynomial from Example 4.4 of [KS 2008] given in free (nonsymmetric) variables.

Example 3.1. Let X denote a single free variable and set

$$M_0 := 3X^4 - 3(XX^*)^2 - 4X^5X^* - 2X^3X^{*3} + 2X^2X^*XX^{*2} + 2X^2X^{*2}XX^* + 2(XX^*)^3.$$

Then the noncommutative Motzkin polynomial is

$$M := 1 + M_0 + M_0^* \in \operatorname{Sym} k\langle X, X^*\rangle.$$

It is trace-nonnegative everywhere since

$$M' := YZ^4Y + ZY^4Z - 3YZ^2Y + 1 \overset{\text{cyc}}{\sim} M\left(\frac{Y + \mathbb{i}Z}{2}, \frac{Y - \mathbb{i}Z}{2}\right) \in k\langle Y, Z\rangle$$

is trace-nonnegative on symmetric matrices; see Example 4.4 of [KS 2008]. Alternatively, $M(X^3, (X^*)^3) \in \Theta^2 k\langle X, X^*\rangle$. On the other hand, $M \notin \Theta^2 k\langle X, X^*\rangle$. (Some of these computations were done with the aid of the computer algebra systems NCSOStools [Cafuta et al. 2010] and NCAlgebra [Helton et al. 2010].)

Connes' embedding conjecture [1976, Section V, pp. 105–107] states that every separable II_1-factor is embeddable in an ultrapower of the hyperfinite II_1-factor. Understanding trace-positive polynomials in the dimension-free setting is the key to this problem, because it is equivalent, by Theorem 1.6 of [KS 2008], to Conjecture 1.5 of the same reference, which we repeat here for convenience:

Conjecture 3.2 (algebraic version of Connes' conjecture). For $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$ the following are equivalent:

(i) $\operatorname{tr}\big(f(\underline{A}, \underline{A}^*)\big) \geq 0$ for all $d \in \mathbb{N}$ and all tuples of contractions $\underline{A} \in \mathrm{M}_d(k)^n$;

(ii) for every $\varepsilon \in \mathbb{R}_{>0}$, $f + \varepsilon$ is cyclically equivalent to an element of the form

$$\sum_j s_j^* s_j + \sum_{i,j} p_{ij}^*(1 - X_i^* X_i) p_{ij},$$

where $s_j, p_{ij} \in k\langle \underline{X}, \underline{X}^*\rangle$.

In the sequel we indicate an approach to this problem "from below". That is, we abandon the dimension-free setting and solve a Hilbert 17-type problem characterizing polynomials with nonnegative trace in a dimension-dependent setting. It is our belief that this might constitute an important step towards (a positive or negative resolution of) Connes' embedding conjecture.

4. Dimension-dependent positivity

The properties (A) and (B) for free algebras in a dimension-dependent setting are well understood due to our previous work. Roughly speaking, a trace-zero polynomial is cyclically equivalent to a polynomial identity [Brešar and Klep 2009, Section 4], and a positive semidefinite polynomial is a sum of Hermitian squares with denominators and weights [Klep and Unger 2010, Section 5]. In this section property (C) is explored and we present our main result, a Positivstellensatz characterizing polynomials with nonnegative trace on all tuples of $d \times d$ matrices for *fixed* d. This is done in Section 4C. Before that we recall generic matrices and universal division algebras with involution in Section 4A and take a look at polynomial preservers of the various notions of positivity in Section 4B.

4A. ***Generic matrices and universal division algebras.*** We assume the reader is familiar with the theory of polynomial identities as presented, e.g., in [Procesi 1973; Rowen 1980]. We review the notion of generic matrices and universal division algebras with involution and refer the reader to [Procesi 1976; Procesi and Schacher 1976] for details.

Let $\zeta := (\zeta_{ij}^{(\ell)} \mid 1 \le i, j \le d,\ 1 \le \ell \le n)$ and $\bar{\zeta} := (\bar{\zeta}_{ij}^{(\ell)} \mid 1 \le i, j \le d,\ 1 \le \ell \le n)$ denote commuting variables. To keep the notation uniform, let

$$\underline{\zeta} := \begin{cases} \zeta & \text{if } k = \mathbb{R}, \\ (\zeta, \bar{\zeta}) & \text{if } k = \mathbb{C}. \end{cases}$$

Form the polynomial $*$-algebra $k[\underline{\zeta}]$ that endowed with the involution that extends complex conjugation on k and fixes $\zeta_{ij}^{(\ell)}$ pointwise (if $k = \mathbb{R}$) or sends $\zeta_{ij}^{(\ell)}$ to $\bar{\zeta}_{ij}^{(\ell)}$ (if $k = \mathbb{C}$).

Consider the $d \times d$ matrices

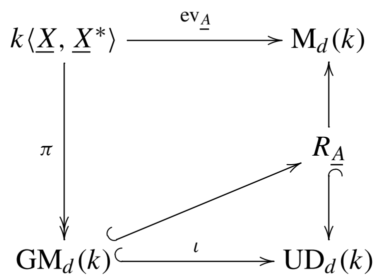
$$Y_\ell := \big[\zeta_{ij}^{(\ell)}\big]_{1 \le i, j \le d} \in \mathrm{M}_d(k[\underline{\zeta}]) \quad \text{for } \ell \in \mathbb{N}.$$

Each Y_ℓ is called a *generic matrix*. The (unital) k-subalgebra of $\mathrm{M}_d(k[\underline{\zeta}])$ generated by the Y_ℓ and their (complex conjugate) transposes is the *ring of generic matrices with involution* $\mathrm{GM}_d(k)$. Equivalently,

$$\mathrm{GM}_d(k) \cong k\langle \underline{X}, \underline{X}^* \rangle / \mathfrak{t}_d,$$

where $\mathfrak{t}_d \subseteq k\langle \underline{X}, \underline{X}^* \rangle$ is the T-ideal of polynomial identities for $d \times d$ matrices.

For $d \ge 2$, the ring $\mathrm{GM}_d(k)$ is a prime PI algebra (see [Procesi and Schacher 1976, Section II]). Hence its central localization is a central simple algebra $\mathrm{UD}_d(k)$ with involution, which we call (by an abuse of notation) the *universal division algebra*. Relating these notions to $*$-representations of the free $*$-algebra is the following commutative diagram: for $d \in \mathbb{N}$ and $\underline{A} \in \mathrm{M}_d(k)^n$, let $R_{\underline{A}}$ denote all the elements of $\mathrm{UD}_d(k)$ that are regular at $\underline{A}$. Then:



For a more geometric viewpoint of the ring of generic matrices and the universal division algebra we refer the reader to [Procesi 1976; Saltman 1999]. The standard textbook on central simple algebras with involution is [Knus et al. 1998].

4B. ***Polynomial preservers.*** In this subsection we present versions of Lemmas 2.1–2.4 in the context of free $*$-algebras. To avoid trivialities, we assume throughout that $d \geq 2$.

Lemma 4.1. *Suppose $f \in k\langle \underline{X}, \underline{X}^*\rangle$ is such that for all $g \in k\langle \underline{X}, \underline{X}^*\rangle$,*

$$g \succeq 0 \text{ on } d \times d \text{ matrices} \quad \Rightarrow \quad fg \succeq 0 \text{ on } d \times d \text{ matrices.} \tag{7}$$

Then f is a central polynomial positive semidefinite on $d \times d$ matrices.

Proof. Using (7) with $g = 1$, we see f is positive semidefinite on $d \times d$ matrices. Thus there is no harm in assuming $f = f^*$.

Again by (7), $fg - gf$ vanishes on all $d \times d$ matrices for all polynomials g of the form $g = h^*h$. That is, $[f, g]$ is a polynomial identity of $d \times d$ matrices. Now the same holds true for all symmetric g, since

$$2[f, g] + [f, g^2] = [f, (1+g)^2]$$

is then a polynomial identity. Hence f commutes (modulo the T-ideal of identities) with all symmetric polynomials.

Every element of $\mathrm{UD}_d(k)$ can be represented as rs^{-1} for some $r, s \in \mathrm{GM}_d(k)$ with $s = s^* \in Z(\mathrm{GM}_d(k))$. Such an element is symmetric if and only if $r = r^*$. So $\pi(f)$ commutes with all symmetric elements of $\mathrm{UD}_d(k)$. By Dieudonné's theorem [1952, Lemma 1], the latter generate $\mathrm{UD}_d(k)$. Hence $\pi(f) \in Z(\mathrm{UD}_d(k))$ and f is indeed a central polynomial.

(Note: once we have established that f commutes with all symmetric polynomials, an easier argument is available if $k = \mathbb{C}$. In this case one immediately obtains that f also commutes with all skew symmetric polynomials as these are all of the form $\mathrm{i}g$ for symmetric g.) □

Lemma 4.2. *Suppose $f \in k\langle \underline{X}, \underline{X}^*\rangle$ is such that for all $g \in k\langle \underline{X}, \underline{X}^*\rangle$,*

$$\text{tr}(g) = 0 \text{ on } d \times d \text{ matrices} \quad \Rightarrow \quad \text{tr}(fg) = 0 \text{ on } d \times d \text{ matrices.} \tag{8}$$

Then f is a central polynomial.

Proof. Let $g = [h_1, h_2]$ for some $h_i \in k\langle \underline{X}, \underline{X}^*\rangle$. Then

$$fg = f[h_1, h_2] = [f, h_1h_2] + [h_1, fh_2] + h_1[h_2, f]. \tag{9}$$

Since $\text{tr}(g) = 0$ on all $d \times d$ matrices, this implies $\text{tr}(h_1[h_2, f]) = 0$ on $d \times d$ matrices. Fix h_2 and denote $r := [h_2, f]$. Then r satisfies

$$\text{tr}(pr) = 0 \text{ on } d \times d \text{ matrices}$$

for all $p \in k\langle \underline{X}, \underline{X}^*\rangle$. Taking $p = -r^*$ leads to $-\text{tr}(r^*r) = 0$, and hence $r = 0$ on all $d \times d$ matrices. That is, r is an identity of $d \times d$ matrices. As $r = [h_2, f]$ and h_2 was arbitrary, this implies f is a central polynomial. □

Lemma 4.3. *Suppose $f \in k\langle \underline{X}, \underline{X}^*\rangle$ is such that for all $g \in k\langle \underline{X}, \underline{X}^*\rangle$,*

$$\text{tr}(g) \geq 0 \text{ on } d \times d \text{ matrices} \quad \Rightarrow \quad \text{tr}(fg) \geq 0 \text{ on } d \times d \text{ matrices.} \tag{10}$$

Then f is a central polynomial positive semidefinite on $d \times d$ matrices.

Proof. If $\text{tr}(g) = 0$, then by (10), $\text{tr}(fg) \geq 0$ and $\text{tr}(-fg) \geq 0$ on $d \times d$ matrices. That is, $\text{tr}(fg) = 0$. Now by Lemma 4.2, f is a central polynomial.

Applying (10) with $g=1$ yields $f(\underline{A}, \underline{A}^*) = \text{tr}\big(f(\underline{A}, \underline{A}^*)\big) \geq 0$ for all $\underline{A} \in \text{M}_d(k)^n$, showing f is positive semidefinite on $d \times d$ matrices. □

Likewise we can characterize polynomials that map positive semidefinite polynomials into trace-nonnegative ones. At the same time this indicates how to build examples of trace-nonnegative polynomials. As we shall see in the next subsection, the procedure is essentially exhaustive.

Lemma 4.4. *Suppose $f \in \text{Sym}\, k\langle \underline{X}, \underline{X}^*\rangle$ is such that for all $g \in k\langle \underline{X}, \underline{X}^*\rangle$,*

$$g \succeq 0 \text{ on } d \times d \text{ matrices} \quad \Rightarrow \quad \text{tr}(fg) \geq 0 \text{ on } d \times d \text{ matrices.} \tag{11}$$

Then f is positive semidefinite on $d \times d$ matrices.

Proof. Assume f is not positive semidefinite on $d \times d$ matrices. Then there exists an n-tuple $\underline{A} = (A_1, \dots, A_n) \in \text{M}_d(k)^n$ with

$$f(\underline{A}, \underline{A}^*) \not\succeq 0. \tag{12}$$

Let $\mathscr{A} \subseteq \text{M}_d(k)$ denote the $*$-subalgebra generated by the $A_1, \dots, A_n$. Since the Hermitian square of a nonzero matrix is not nilpotent, $\mathscr{A}$ is semisimple. By the Artin–Wedderburn theorem, $\mathscr{A}$ is $*$-isomorphic to a direct sum of full matrix algebras. We distinguish two cases.

CASE 1: If $k = \mathbb{C}$, there is a $*$-isomorphism

$$\mathscr{A} \cong \bigoplus_{j=1}^{s} \mathrm{M}_{d_j}(\mathbb{C}) \tag{13}$$

for some $d_j \in \mathbb{C}$, and $\sum_j d_j \leq d$. This induces a block diagonalization

$$A_j = \begin{bmatrix} A_{j,1} & & \\ & \ddots & \\ & & A_{j,s} \end{bmatrix}, \quad \text{with } A_{j,k} \in \mathrm{M}_{d_k}(\mathbb{C}).$$

By (12), there is a j such that $\underline{A}_{(j)} = (A_{1,j}, \ldots, A_{n,j}) \in \mathrm{M}_{d_j}(\mathbb{C})^n$ satisfies

$$f(\underline{A}_{(j)}, \underline{A}^*_{(j)}) \not\succeq 0.$$

Choose $u \in \mathbb{C}^{d_j}$ with

$$\big\langle f(\underline{A}_{(j)}, \underline{A}^*_{(j)})u, u\big\rangle < 0. \tag{14}$$

There is a $B \in \mathrm{M}_{d_j}(\mathbb{C})$ with $Be_{i,d_j} = u$ for all $i = 1, \ldots, d_j$. (Here e_{i,d_j} are the standard basis vectors for $\mathbb{C}^{d_j}$.) By the construction of $\mathscr{A}$ and (13), there is an $h \in \mathbb{C}\langle \underline{X}, \underline{X}^*\rangle$ with $h(\underline{A}_{(j)}, \underline{A}^*_{(j)}) = B$. Let $g = hh^*$. Then

$$\begin{aligned} \operatorname{tr}((fg)(\underline{A}_{(j)}, \underline{A}^*_{(j)})) &= \operatorname{tr}((h^* f h)(\underline{A}_{(j)}, \underline{A}^*_{(j)})) \\ &= \sum_{i=1}^{d_j} \big\langle h^*(\underline{A}_{(j)}, \underline{A}^*_{(j)}) f(\underline{A}_{(j)}, \underline{A}^*_{(j)}) h(\underline{A}_{(j)}, \underline{A}^*_{(j)}) e_{i,d_j}, e_{i,d_j}\big\rangle \\ &= \sum_{i=1}^{d_j} \big\langle f(\underline{A}_{(j)}, \underline{A}^*_{(j)}) Be_{i,d_j}, Be_{i,d_j}\big\rangle \\ &= \sum_{i=1}^{d_j} \big\langle f(\underline{A}_{(j)}, \underline{A}^*_{(j)})u, u\big\rangle < 0. \end{aligned} \tag{15}$$

As this contradicts our assumption (11), we conclude that $f \succeq 0$ on $d \times d$ matrices.

CASE 2: If $k = \mathbb{R}$, the reasoning is the same with a minor technical modification. Let

$$\mathscr{A} \cong \bigoplus_{j=1}^{s} \mathrm{M}_{d_j}(\mathbb{R}) \oplus \bigoplus_{k=1}^{r} \mathrm{M}_{e_k}(\mathbb{C}) \oplus \bigoplus_{\ell=1}^{p} \mathrm{M}_{f_\ell}(\mathbb{H}) \tag{16}$$

for some $d_j, e_k, f_\ell \in \mathbb{N}$.

If there is a tuple $\underline{A} \in \mathrm{M}_{d_j}(\mathbb{R})^n$ with $f(\underline{A}, \underline{A}^*) \not\succeq 0$, we proceed as in Case 1. If there is an $\underline{A} \in \mathrm{M}_{e_k}(\mathbb{C})^n$ with $0 \not\preceq f(\underline{A}, \underline{A}^*) \in \mathrm{M}_{e_k}(\mathbb{C})$, we proceed as follows. Let V be the invariant subspace of $\mathbb{R}^d$ corresponding to the action of $\mathrm{M}_{e_k}(\mathbb{C})$. There is a $u \in V$ with $\langle f(\underline{A}, \underline{A}^*)u, u\rangle < 0$. Pick a basis $\{v_1, \ldots, v_{e_k}\}$ of V over $\mathbb{C}$, and let

$B \in \mathrm{M}_{e_k}(\mathbb{C})$ satisfy $Bv_j = u$ for all j. Choose $h \in \mathbb{R}\langle \underline{X}, \underline{X}^* \rangle$ with $h(\underline{A}, \underline{A}^*) = B$ and $g = hh^*$. Then the *complex* trace z of $(fg)(\underline{A}, \underline{A}^*)$ is negative by the same computation as in (15). Hence the *real* trace satisfies

$$\operatorname{tr}\big((fg)(\underline{A}, \underline{A}^*)\big) = \frac{z+\bar{z}}{2} < 0.$$

The remaining case of quaternion matrices is dealt with similarly. We leave this as an exercise for the reader. □

It is clear that converses of Lemmas 4.1–4.4 hold true. Also, with the exception of (11), which is satisfied when f is a sum of Hermitian squares, there are no nonconstant dimension-free polynomial preservers.

4C. ***The dimension-dependent tracial Positivstellensatz.*** Our main tool for describing trace-nonnegative polynomials is the following proposition deduced from the properties of the reduced trace [Knus et al. 1998, Section 1] on $\mathrm{UD}_d(k)$.

Proposition 4.5. *For every $f \in k\langle \underline{X}, \underline{X}^* \rangle$ and $d \in \mathbb{N}$ there exists a nonvanishing central polynomial for $d \times d$ matrices, denoted by $c \in k\langle \underline{X}, \underline{X}^* \rangle$, such that cf is cyclically equivalent to a central polynomial. That is,*

$$cf \overset{\text{cyc}}{\sim} c' \tag{17}$$

for some central polynomial c'.

Proof. Consider $F := \iota(\pi(f)) \in \mathrm{UD}_d(k)$. So $\mathrm{Trd}(F) \in Z(\mathrm{UD}_d(k))$, and there is a nonvanishing central polynomial $c_0 \in k\langle \underline{X}, \underline{X}^* \rangle$ and a central polynomial c_0' with

$$\mathrm{Trd}(F) = \pi(c_0')\pi(c_0)^{-1}. \tag{18}$$

Since Trd is $Z(\mathrm{UD}_d(k))$-linear, this yields $\mathrm{Trd}(\pi(c_0 f - c_0')) = 0$. By [Amitsur and Rowen 1994, Theorem 2.4], $\pi(c_0 f - c_0') \overset{\text{cyc}}{\sim} 0$ in $\mathrm{UD}_d(k)$. Clearing denominators shows

$$\pi(cf - c'') \overset{\text{cyc}}{\sim} 0 \tag{19}$$

in $\mathrm{GM}_d(k)$ for a nonvanishing central polynomial c and a central polynomial c''. Lifting (19) to $k\langle \underline{X}, \underline{X}^* \rangle$ gives the desired conclusion: $cf \overset{\text{cyc}}{\sim} c'$. □

Remark 4.6. Instead of the Amitsur–Rowen result used in this proof, we can apply the tracial Nullstellensatz [Brešar and Klep 2009, Theorem 5.2]: once we have established that $\mathrm{Trd}(\pi(c_o f - c_0')) = 0$, by clearing denominators we obtain $\mathrm{tr}(\pi(c_0 c'' f - c_0' c'')) = 0$ for some nonvanishing central polynomial c''. Hence $\pi(c_0 c'' f - c' c'') \overset{\text{cyc}}{\sim} 0$ in $\mathrm{GM}_d(k)$ by [Brešar and Klep 2009, Theorem 5.2]. As before, lifting this relation to $k\langle \underline{X}, \underline{X}^* \rangle$ yields the desired conclusion.

We are now ready to give our main results characterizing trace-nonnegative polynomials.

Theorem 4.7. *Let $k \in \{\mathbb{R}, \mathbb{C}\}$ and suppose $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$ satisfies*

$$\operatorname{tr}\bigl(f(\underline{A}, \underline{A}^*)\bigr) \geq 0 \tag{20}$$

for all $\underline{A} \in \mathrm{M}_d(k)^n$. Then there is a nonvanishing central polynomial for $d \times d$ matrices, denoted by $c \in k\langle \underline{X}, \underline{X}^*\rangle$, such that cfc^* is cyclically equivalent to a polynomial $g \in k\langle \underline{X}, \underline{X}^*\rangle$ that is positive semidefinite on $d \times d$ matrices:

$$cfc^* \overset{\mathrm{cyc}}{\sim} g \quad \text{and} \quad g \succeq 0 \text{ on } d \times d \text{ matrices.} \tag{21}$$

Proof. This is a consequence of Proposition 4.5. Indeed, there is a nonvanishing central polynomial c with

$$cf \overset{\mathrm{cyc}}{\sim} c' \tag{22}$$

for a central polynomial c'. Multiplying (22) with c^* (from the right) shows

$$cfc^* \overset{\mathrm{cyc}}{\sim} c'c^*. \tag{23}$$

For any $\underline{A} \in \mathrm{M}_d(k)^n$,

$$\begin{aligned} 0 \leq \operatorname{tr}\bigl(c(\underline{A}, \underline{A}^*)f(\underline{A}, \underline{A}^*)c(\underline{A}, \underline{A}^*)^*\bigr) &= \operatorname{tr}\bigl(c'(\underline{A}, \underline{A}^*)c(\underline{A}, \underline{A}^*)^*\bigr) \\ = \operatorname{tr}\bigl((c'c^*)(\underline{A}, \underline{A}^*)\bigr) &= (c'c^*)(\underline{A}, \underline{A}^*). \end{aligned} \tag{24}$$

So $g := c'c^*$ is a (central) polynomial positive semidefinite on $d \times d$ matrices satisfying

$$cfc^* \overset{\mathrm{cyc}}{\sim} g. \qquad \square$$

Remark 4.8. The proof shows that g in Theorem 4.7 can actually be taken to be a central polynomial.

Combining Theorem 4.7 with the dimension-dependent Positivstellensatz for positive semidefinite polynomials ([Procesi and Schacher 1976, Theorem 5.4] or [Klep and Unger 2010, Theorem 5.4]) yields:

Corollary 4.9. *Choose $\alpha_1, \dots, \alpha_m \in k\langle \underline{X}, \underline{X}^*\rangle$ whose images in $\mathrm{GM}_d(k)$ form a diagonalization of the quadratic form $\operatorname{Trd}(x^*x)$ on $\mathrm{UD}_d(k)$. For $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$, the following are equivalent*:

(i) $\operatorname{tr}\bigl(f(\underline{A}, \underline{A}^*)\bigr) \geq 0$ *for every $\underline{A} \in \mathrm{M}_d(k)^n$.*

(ii) *There exists a nonvanishing central polynomial $c \in k\langle \underline{X}, \underline{X}^*\rangle$, a polynomial identity $h \in k\langle \underline{X}, \underline{X}^*\rangle$ for $d \times d$ matrices, and $p_{i,\varepsilon} \in k\langle \underline{X}, \underline{X}^*\rangle$ with*

$$cfc^* \overset{\mathrm{cyc}}{\sim} h + \sum_{\varepsilon \in \{0,1\}^m} \underline{\alpha}^{\varepsilon} \sum_i p_{i,\varepsilon}^* p_{i,\varepsilon}. \tag{25}$$

Remark 4.10. For experts we mention that, by applying the reduced trace, we can reformulate (25) as

$$cfc^* \overset{\text{cyc}}{\sim} h+t, \tag{26}$$

where c and h are as above, and t belongs to the preordering in $Z(\mathrm{UD}_d(k))$ generated by the α_j.

If $d=2$, the weights α_j are superfluous since the reduced trace of a Hermitian square is a sum of Hermitian squares in this case (see [Procesi and Schacher 1976, p. 405] or [Klep and Unger 2010, Section 4]), and Corollary 4.9 simplifies as follows:

Corollary 4.11. *For $f \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$, the following are equivalent*:

(i) $\operatorname{tr}\big(f(\underline{A}, \underline{A}^*)\big) \geq 0$ *for every* $\underline{A} \in \mathrm{M}_2(k)^n$.

(ii) *There exists a nonvanishing central polynomial $c \in k\langle \underline{X}, \underline{X}^*\rangle$, and a polynomial identity $h \in k\langle \underline{X}, \underline{X}^*\rangle$ for 2×2 matrices, such that*

$$cfc^* \in h + \Theta^2\, k\langle \underline{X}, \underline{X}^*\rangle. \tag{27}$$

Example 4.12. We finish this presentation with an example showing denominators are necessary for these results to hold. First, the Motzkin polynomial M from Example 3.1 is not cyclically equivalent to a sum of Hermitian squares modulo a T-ideal of identities. Indeed, suppose that

$$M \overset{\text{cyc}}{\sim} h + \sum g_j^* g_j \tag{28}$$

for some $g_j \in k\langle \underline{X}, \underline{X}^*\rangle$ and a polynomial identity $h \in k\langle \underline{X}, \underline{X}^*\rangle$ for $d\times d$ matrices ($d \geq 2$). Then

$$M_{\text{cc}} = \operatorname{tr}\left(M\left(\begin{bmatrix} Y/2 & Z/2 \\ -Z/2 & Y/2\end{bmatrix}\right)\right) = \sum \operatorname{tr}\left((g_j^* g_j)\left(\begin{bmatrix} Y/2 & Z/2 \\ -Z/2 & Y/2\end{bmatrix}\right)\right),$$

where $M_{\text{cc}} \in \mathbb{R}[Y, Z]$ denotes the commutative collapse $Y^4Z^2+Y^2Z^4-3Y^2Z^2+1$ of the noncommutative variant M' of the Motzkin polynomial (in symmetric variables). Since M_{cc} is not a sum of squares in $\mathbb{R}[Y, Z]$, and the trace of a Hermitian square is a sum of squares, M does not satisfy a relation of the form (28). Hence a denominator is needed in Corollaries 4.9 and 4.11.

A little more work is required to show the necessity of the denominator in Theorem 4.7. Let $d \in \mathbb{N}$ be sufficiently large (at least 127, the dimension of the vector space of all polynomials in X, X^* of degree at most 6). Suppose M is cyclically equivalent to a polynomial g that is positive semidefinite on $d\times d$ matrices. Without loss of generality, $g \in \operatorname{Sym} k\langle \underline{X}, \underline{X}^*\rangle$. Choose g of the smallest possible degree. If this degree is greater than 6, then the highest homogeneous component $g^{(\infty)}$ of g is positive semidefinite on $d\times d$ matrices and at the same time $g^{(\infty)} \overset{\text{cyc}}{\sim} 0$. Hence $\operatorname{tr}(g^{(\infty)}) = 0$ on $d \times d$ matrices, implying that $g^{(\infty)}$ is a polynomial identity. Then

$$M \overset{\text{cyc}}{\sim} (g - g^{(\infty)}),$$

with $g - g^{(\infty)}$ positive semidefinite and of degree smaller than g. This contradicts the minimality of g, so $\deg(g) \leq 6$.

Now g is positive semidefinite on $d \times d$ matrices for some $d \geq 127$ and is thus a sum of Hermitian squares by Helton's sum of squares theorem [2002]. But M is not cyclically equivalent to a sum of Hermitian squares by the first part of this example.

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