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Globally trace-positive noncommutative polynomials and the unbounded tracial moment problem

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Abstract

A noncommutative (nc) polynomial is called (globally) trace-positive if its evaluation at any tuple of operators in a tracial von Neumann algebra has nonnegative trace. Such polynomials emerge as trace inequalities in several matrix or operator variables, and are widespread in mathematics and physics. This paper delivers the first Positivstellensatz for global trace positivity of nc polynomials. Analogously to Hilbert's 17th problem in real algebraic geometry, trace-positive nc polynomials are shown to be weakly sums of hermitian squares and commutators of regular nc rational functions. In two variables, this result is strengthened further using a new sum-of-squares certificate with concrete univariate denominators for nonnegative bivariate polynomials. The trace positivity certificates in this paper are obtained by convex duality through solving the so-called unbounded tracial moment problem, which arises from noncommutative integration theory and free probability. Given a linear functional on nc polynomials, the tracial moment problem asks whether it is a joint distribution of integral operators affiliated with a tracial von Neumann algebra. A counterpart to Haviland's theorem on solvability of the tracial moment problem is established. Moreover, a variant of Carleman's condition is shown to guarantee the existence of a solution to the tracial

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moment problem. Together with semidefinite optimization, this is then used to prove that every trace-positive nc polynomial admits an explicit approximation in the 1-norm on its coefficients by sums of hermitian squares and commutators of nc polynomials.

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1 Introduction

Trace inequalities in several operator variables are ubiquitous in mathematics and physics. For example, Golden–Thompson, Lieb–Thirring inequalities and their generalizations play an important role in quantum statistical mechanics [7, 54]. Another source of trace inequalities is quantum information [3, 41], where they materialize through data processing inequalities and restrictions on quantum correlations. In operator algebras [15, 39] and noncommutative probability [18, 24], they appear through Hölder, Minkowski and other inequalities in noncommutative L^p-spaces, as well as trace convexity of entropy. In mathematical optimization, hierarchies of semidefinite programs based on tracial noncommutative optimization are applied to compute matrix factorization ranks [16]. Finally, the recently resolved [23] Connes' embedding problem has several interpretations in terms of trace inequalities [19, 28, 40, 45]. This paper studies trace polynomial inequalities that are valid globally, without restrictions on the variables or their norms, in all finite von Neumann algebras. For the first time, we provide necessary and sufficient certificates (Positivstellensätze) for such inequalities to hold, obtained by solving the associated unconstrained tracial moment problem.

Let $\mathbb{R}\langle \underline{x}\rangle$ be the real free $*$-algebra of noncommutative (nc) polynomials in self-adjoint variables $x_1, \ldots, x_n$. A tracial von Neumann algebra is a pair $(\mathcal{F}, \tau)$ consisting of a finite von Neumann algebra $\mathcal{F}$ and a tracial state τ on $\mathcal{F}$. Given an nc polynomial $f \in \mathbb{R}\langle \underline{x}\rangle$ and a tuple of self-adjoint operators $\underline{X} \in \mathcal{F}_{\mathrm{sa}}^n$, we consider the evaluation $f(\underline{X}) \in \mathcal{F}$ and its trace $\tau(f(\underline{X})) \in \mathbb{C}$. We say that $f \in \mathbb{R}\langle \underline{x}\rangle$ is **(globally) trace-positive** if $\tau(f(\underline{X})) \geq 0$ for all $\underline{X} \in \mathcal{F}_{\mathrm{sa}}^n$ and all tracial von Neumann algebras $(\mathcal{F}, \tau)$.

The notion of trace positivity of nc polynomials fits in between positivity (of commutative polynomials) on tuples of real numbers and positive semidefiniteness on tuples of operators. Commutative and operator positivity are both well-studied, the former in real algebraic geometry and moment problems [11, 35, 49, 53], and the latter under the umbrella of free analysis and free convexity [1, 17, 21]. In both cases, algebraic certificates for positivity, the so-called Positivstellensätze, are usually given in terms of sums of squares. For example, the famous resolution of Hilbert's 17th problem asserts that a commutative polynomial is nonnegative if and only if it is a sum of squares of *rational* functions. Analogously, an nc polynomial is everywhere positive semidefinite if and only if it is a sum of hermitian squares of nc polynomials [20, 36]. On the other hand, results on trace-positive nc polynomials are scarcer. Only algebraic certificates for trace positivity on domains with additional restrictions have been given so far. In [25, 28], Positivstellensätze for trace positivity on bounded domains (in terms of Archimedean quadratic modules) were derived. Likewise well-understood are nc polynomials that are trace-positive on tuples of $k \times k$ matrices for a fixed $k \in \mathbb{N}$

[29], which were focal in the Procesi–Schacher conjecture [42]. On the other hand, a characterization of nc polynomials that are trace-positive without norm or dimension restrictions on the input has been absent (except for the single operator case, where even positivity of polynomials in trace powers can be handled [27]).

Polynomial positivity is dual to moment problems [11, 43, 53]. While the classical moment problem aims at determining which functionals on a polynomial ring arise from integration with respect to some measure, the tracial moment problem considers functionals on a free algebra that arise from noncommutative integration [38] with respect to a trace on a von Neumann algebra. Its C^*-analog pertains to relativistic quantum theory [12]. In free probability, a unital algebra $\mathcal{A}$ with a trace τ is viewed as a noncommutative probability space, and the functionals on $\mathbb{R}\langle \underline{x} \rangle$ of the form $p \mapsto \tau(p(\underline{X}))$ for $\underline{X} \in \mathcal{A}^n$ are called noncommutative laws or joint distributions of $\underline{X}$ [37, 57]. Noncommutative joint distributionsgiven by evaluations on tuples of elements from tracial von Neumann algebras $(\mathcal{F}, \tau)$ have been characterized by the solution of the bounded tracial moment problem [19, 45]. The special case of noncommutative joint distributionsof tuples from finite-dimensional von Neumann algebras is settled in [6]. This paper solves the unbounded tracial moment problem of describing functionals arising from τ and evaluations on (possibly unbounded) operators affiliated with $\mathcal{F}$.

1.1 Main results

The contribution of this paper is twofold: we solve the unbounded tracial moment problem, and derive a Positivstellensatz for trace-positive nc polynomials. Before stating these results, we require some notation. Given a tracial von Neumann algebra $(\mathcal{F}, \tau)$, let $L^\omega(\mathcal{F}, \tau)$ be its $*$-algebra of power-integrable operators, i.e., the intersection of all the L^p-spaces associated with $(\mathcal{F}, \tau)$. That is, $X \in L^\omega(\mathcal{F}, \tau)$ if X is an operator affiliated with $\mathcal{F}$, and $\tau(|X|^p) < \infty$ for all $p \in \mathbb{N}$. Let $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ be the subspace of symmetric (or self-adjoint) polynomials in $\mathbb{R}\langle \underline{x} \rangle$. Obvious examples of trace-positive polynomials are sums of hermitian squares and commutators of nc polynomials; however, not all trace-positive polynomials are of this form. To remedy this, one has to replace nc polynomials with a certain class of regular nc rational functions. Let $\mathcal{K} \subset \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ be the convex cone of all (symmetric) nc polynomials that can be written as sums of hermitian squares and commutators of elements in the $*$-subalgebra

$$\mathbb{R}\langle x_1, \ldots, x_n, (1 + x_1^2)^{-1}, \ldots, (1 + x_n^2)^{-1} \rangle$$

of the free skew field [9, 58]. For example, the following noncommutative lift of the Motzkin polynomial

$$x_2 x_1^4 x_2 + x_2^2 x_1^2 x_2^2 - 3 x_2 x_1^2 x_2 + 1$$

belongs to $\mathcal{K}$ (Example 3.2) even though it is not a sum of hermitian squares and commutators of nc polynomials. The cone $\mathcal{K}$ plays a central role in our first main result, the solution of the unbounded tracial moment problem. The following theorem comprises tracial analogs of Haviland's theorem and Carleman's condition.

Theorem A *Let $\varphi : \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \to \mathbb{R}$ be a linear functional with $\varphi(1) = 1$.*

(a) *There exists a tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in L^\omega(\mathcal{F}, \tau)^n$ such that $\varphi(p) = \tau(p(\underline{X}))$ for all $p \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ if and only if $\varphi(\mathcal{K}) = \mathbb{R}_{\geq 0}$.*
(b) *The equivalent conditions in (a) hold if there is $M > 0$ such that $\varphi(x_j^r) \leq r! M^r$ for all $j = 1, \ldots, n$ and even $r \in \mathbb{N}$.*

The first part of Theorem A is proved as Theorem 4.2, while the second part is given in Theorem 7.1. The proof combines methods and results from convexity [2], the theory of unbounded operators [52], and noncommutative integration [38, 55]. Theorem A is used to obtain a tracial Positivstellensatz for nc polynomials.

Theorem B *The following are equivalent for $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$:*

(i) *$\tau(f(\underline{X})) \geq 0$ for all $(\mathcal{F}, \tau)$ and $\underline{X} \in \mathcal{F}^n$;*
(ii) *$\tau(f(\underline{X})) \geq 0$ for all $(\mathcal{F}, \tau)$ and $\underline{X} \in L^\omega(\mathcal{F}, \tau)^n$;*
(iii) *f lies in the closure of $\mathcal{K}$ with respect to the finest locally convex topology on $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$;*
(iv) *for every $\varepsilon > 0$ there exists $r \in \mathbb{N}$ such that*

$$f + \varepsilon \sum_{j=1}^{n} \sum_{k=0}^{r} \frac{1}{k!} x_j^{2k}$$

is a sum of hermitian squares and commutators in $\mathbb{R}\langle \underline{x} \rangle$.

See Theorems 6.1 and 7.2 below for the proof. In addition to the aforementioned mathematics areas, techniques from polynomial and semidefinite optimization [6, 31] are applied in the proof of Theorem B.

The negative answer to Connes' embedding problem [23] implies that in general, one cannot restrict (i) in Theorem B to finite-dimensional von Neumann algebras (Proposition 6.4). Nevertheless, it suffices to consider only II_1 factors in Theorem B(i). On the other hand, trace polynomial inequalities that are valid in all finite von Neumann algebras (and are described by Theorem B) do not necessarily hold in all formal tracial algebras [39].

Alas, the cone $\mathcal{K}$ is not closed in general (Proposition 6.8). However, the statement of Theorem B can be improved for a class of bivariate nc polynomials. We say that $f \in \mathbb{R}\langle x_1, x_2 \rangle$ is *cyclically sorted* if it is a linear combination of cyclic permutations of products of the form $x_1^i x_2^j$. It turns out (Corollary 5.4) that cyclically sorted nc polynomials are trace-positive precisely when they belong to $\mathcal{K}$. This statement is a consequence of the following new Positivstellensatz for commutative polynomials.

Theorem C *If $f \in \mathbb{R}[x, y]$ is nonnegative on $\mathbb{R}^2$ then there exists $k \in \mathbb{N}$ such that $(1 + x^2)^k f$ is a sum of squares in $\mathbb{R}[x, y]$.*

The proof (see Theorem 5.2) relies on real algebraic geometry of affine surfaces [49]. Theorem C is a strenghtened solution of Hilbert's 17th problem for bivariate polynomials, since only rational squares with uniform univariate denominators are needed.

2 Preliminaries

In this section we review the terminology and notation on von Neumann algebras, their affiliated operators, nc polynomials and rational functions that are used throughout the paper.

2.1 Affiliated and power-integrable operators

A *tracial von Neumann algebra* is a pair $(\mathcal{F}, \tau)$ of a finite von Neumann algebra $\mathcal{F}$ with a separable predual and a faithful normal tracial state τ on $\mathcal{F}$. Suppose $\mathcal{F}$ acts on a Hilbert space $\mathcal{H}$; then a closed and densely defined operator X on $\mathcal{H}$ is *affiliated with* $\mathcal{F}$ if it commutes with every unitary operator in the commutant of $\mathcal{F}$ in $\mathcal{B}(\mathcal{H})$.

Next we review selected notions from noncommutative integration theory, following [38, 55]. For $p \in [1, \infty)$, the *noncommutative L^p-space* $L^p(\mathcal{F}, \tau)$ is the completion of $\mathcal{F}$ with respect to the norm $X \mapsto \tau(|X|^p)^{1/p}$ [38, Section 3]. Note that $L^2(\mathcal{F}, \tau)$ is a Hilbert space, and $\mathcal{F}$ acts on it via the left regular representation. Since τ is finite, operators on $L^2(\mathcal{F}, \tau)$ affiliated with $\mathcal{F}$ form a $*$-algebra [38, Section 2]: the sum/product of closed affiliated operators are understood as the closure of the sum/product as unbounded operators; see also [55, Section IX.2]. The sequence $(L^p(\mathcal{F}, \tau))_{p\in[1,\infty)}$ can then be naturally seen as a decreasing net of nested subspaces in this algebra of operators affiliated with $\mathcal{F}$ [38, Theorem 5]. Hölder's inequality for noncommutative L^p-spaces [55, Theorem IX.2.13(iv)] states that

$$\left|\tau(Z_1 \cdots Z_n)\right| \leq \|Z_1\|_{p_1} \cdots \|Z_n\|_{p_n} \tag{2.1}$$

for $Z_j \in L^{p_j}(\mathcal{F}, \tau)$ and $\frac{1}{p_1} + \cdots + \frac{1}{p_n} = 1$. Therefore

$$L^{\omega}(\mathcal{F}, \tau) := \bigcap_{p\in[1,\infty)} L^p(\mathcal{F}, \tau)$$

is a $*$-algebra, and τ extends to a tracial state on $L^{\omega}(\mathcal{F}, \tau)$. The algebra $L^{\omega}(\mathcal{F}, \tau)$ was introduced in [22, Section 3], and its elements are *power-integrable operators* affiliated with $(\mathcal{F}, \tau)$. For example, if $\mathcal{F} = L^{\infty}([0, 1])$ and τ is the integration with respect to the Lebesgue measure on $[0, 1]$, then $\log(t) \in L^{\omega}(\mathcal{F}, \tau)\backslash\mathcal{F}$ and $\tau(|\log(t)|^p) = p!$.

2.2 Noncommutative polynomials and rational functions

Let $\underline{x} = (x_1, \ldots, x_n)$ be a tuple of freely noncommuting variables, and let $<\underline{x}>$ be the free monoid of words in $\underline{x}$. Let $\mathbb{R}<\underline{x}>$ be the real free $*$-algebra of *nc polynomials* over $\underline{x}$, with the involution given by $x_j^* = x_j$ for $j = 1, \ldots, n$. For $d \in \mathbb{N}$ let $\mathbb{R}<\underline{x}>_d \subset \mathbb{R}<\underline{x}>$ be the subspace of nc polynomials of degree at most d. The universal skew field of fractions of $\mathbb{R}<\underline{x}>$ is the free skew $*$-field $\mathbb{R}\langle\underline{x}\rangle$ (see e.g. [9, 26, 58]). In this paper, we consider the following $*$-subalgebra of $\mathbb{R}\langle\underline{x}\rangle$:

$$\mathcal{A} := \mathbb{R}<x_1, \ldots, x_n, (1 + x_1^2)^{-1}, \ldots, (1 + x_n^2)^{-1}> .$$

Alternatively, $\mathcal{A}$ can be viewed as the free product of n copies of $\mathbb{R}[t, \frac{1}{1+t^2}]$. For $d \in \mathbb{N}$ let $\mathcal{A}_d \subset \mathcal{A}$ denote the subspace of elements that are linear combinations of products in $x_1, \ldots, x_n, (1+x_1^2)^{-1}, \ldots, (1+x_n^2)^{-1}$ of length at most d.

If $\underline{X}$ is a tuple of (possibly unbounded) self-adjoint operators affiliated with a finite von Neumann algebra $\mathcal{F}$, then the evaluation

$$a(\underline{X}) = a(X_1, \ldots, X_n, (I+X_1^2)^{-1}, \ldots, (I+X_n^2)^{-1})$$

is well-defined for every $a \in \mathcal{A}$ because the affiliated operators form an algebra and $(I+X)^{-1}$ is a bounded operator for a self-adjoint X. Furthermore, if $\underline{X} \in L^\omega(\mathcal{F}, \tau)^n$ then $\tau(a(\underline{X}))$ is well-defined. More precisely, if $a \in \mathcal{A}_p$ then $\tau(a(\underline{X}))$ is well-defined for every $\underline{X} \in L^p(\mathcal{F}, \tau)^n$ by Hölder's inequality (2.1).

3 Sums of hermitian squares with denominators, and the cone $\mathcal{K}$

This section is devoted to the introduction and first properties of the convex cone $\mathcal{K}$ (see (3.1) below) that is essential for the moment problem and positivity certificates of this paper.

Given a $*$-algebra $\mathcal{B}$ let

$$\begin{aligned}
\mathcal{B}_{\mathrm{sa}} &= \{b \in \mathcal{B} \colon b^* = b\},\\
\Sigma^2\mathcal{B} &= \left\{ \sum_i b_i b_i^* \colon b_i \in \mathcal{B} \right\},\\
[\mathcal{B}, \mathcal{B}] &= \operatorname{span}\{b_1 b_2 - b_2 b_1 \colon b_1, b_2 \in \mathcal{B}\}.
\end{aligned}$$

The following lemma lists relations between the above convex cones and subspaces in the $*$-algebras $\mathbb{R}\langle \underline{x} \rangle$ and $\mathcal{A}$.

Lemma 3.1 *Under the natural embedding $\mathbb{R}\langle \underline{x} \rangle \subset \mathcal{A}$,*

(a) $[\mathcal{A}, \mathcal{A}] \cap \mathbb{R}\langle \underline{x} \rangle = [\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle]$;
(b) $\Sigma^2\mathcal{A} \cap \mathbb{R}\langle \underline{x} \rangle = \Sigma^2\mathbb{R}\langle \underline{x} \rangle$;
(c) $\Sigma^2\mathcal{A} \cap [\mathcal{A}, \mathcal{A}] = \{0\}$;
(d) $(\Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}]) \cap \mathbb{R}\langle \underline{x} \rangle \supsetneq \Sigma^2\mathbb{R}\langle \underline{x} \rangle + [\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle]$ *for* $n \geq 2$;
(e) $(1+x_j^2)^{-m}, 1-(1+x_j^2)^{-m} \in \Sigma^2\mathcal{A}$ *for all* $m \in \mathbb{N}$.

Proof (a) There is an embedding of $\mathcal{A}$ into formal power series $\mathbb{R}\langle\langle \underline{x} \rangle\rangle$ that sends $(1+x_j^2)^{-1}$ to $\sum_{k=0}^\infty (-1)^k x_j^{2k}$. If $s, t \in \mathbb{R}\langle\langle \underline{x} \rangle\rangle$ are given as $s = \sum_{w \in \langle \underline{x} \rangle^*} s_w w$ and $t = \sum_{w \in \langle \underline{x} \rangle^*} t_w w$, then their commutator

$$[s,t] = \sum_{i=0}^\infty \sum_{|u|+|v|=i} s_u t_v \cdot [u, v]$$

is a convergent (with respect to the adic topology of the power series) series of commutators. From here we immediately deduce that $[\mathbb{R}\langle\langle \underline{x}\rangle\rangle, \mathbb{R}\langle\langle \underline{x}\rangle\rangle] \cap \mathbb{R}\langle \underline{x}\rangle = [\mathbb{R}\langle \underline{x}\rangle, \mathbb{R}\langle \underline{x}\rangle]$, so (a) follows.

(b) If $\underline{X} \in \mathrm{M}_k(\mathbb{C})^n_{\mathrm{sa}}$ and $s \in \Sigma^2\mathcal{A}$, then $s(\underline{X})$ is a positive semidefinite matrix. Hence (b) holds by the Helton-McCullough Positivstellensatz, see [36, Theorem 0.2] or [20, Theorem 1.1].

(c) For every $\underline{X} \in \mathrm{M}_k(\mathbb{C})^n_{\mathrm{sa}}$ and $c \in [\mathcal{A}, \mathcal{A}]$ we have $\mathrm{tr}(c(\underline{X})) = 0$. On the other hand, if $f \in \mathcal{A}\backslash\{0\}$, then there are $k \in \mathbb{N}$ and $\underline{Y} \in \mathrm{M}_k(\mathbb{C})^n_{\mathrm{sa}}$ such that $f(\underline{Y})$ is nonzero, see e.g. [58, Remark 6.7]. Consequently $\mathrm{tr}(f(\underline{Y})f^*(\underline{Y})) > 0$. Therefore (c) holds.

(d) See Example 3.2 below.

(e) Since $(1+x_j^2)^{-1} = (1+x_j^2)^{-2}(1+x_j^2)$ and $1-(1+x_j^2)^{-1} = x_j^2(1+x_j^2)^{-1}$ belong to $\Sigma^2\mathcal{A}$, so do $(1+x_j^2)^{-m}$ and $1-(1+x_j^2)^{-m} = (1-(1+x_j^2)^{-1})\sum_{i=0}^{m-1}(1+x_j^2)^{-i}$ for every $m \in \mathbb{N}$. □

Example 3.2 Let $m = x_2x_1^4x_2 + x_2^2x_1^2x_2^2 - 3x_2x_1^2x_2 + 1$. Note that m is a noncommutative lift of the classical Motzkin polynomial (see [35, Proposition 1.2.2] or [49, Remark 1.1.2]), which is nonnegative on $\mathbb{R}^2$ but not a sum of squares of polynomials. In particular, $m \notin \Sigma^2\mathbb{R}\langle \underline{x}\rangle + [\mathbb{R}\langle \underline{x}\rangle, \mathbb{R}\langle \underline{x}\rangle]$. On the other hand, by [44, Section 4.2] we have $m = s + c$ for $s \in \Sigma^2\mathcal{A}$ and $c \in [\mathcal{A}, \mathcal{A}]$ where

$$\begin{aligned} s = {} & (1-x_1^2x_2^2)^*(1+x_1^2)^{-1}(1-x_1^2x_2^2) + \\ & x_2(1+x_1^2)^{-1}(x_1^3-x_1)^2x_2 + (x_2^2-1)(1+x_1^2)^{-1}x_1^2(x_2^2-1) \end{aligned}$$

and

$$c = 2\big[x_2, [(1+x_1^2)^{-1}, x_2]\big].$$

Let us define the convex cone

$$\mathcal{K} := \big(\Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}]\big) \cap \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}} \tag{3.1}$$

in $\mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}}$.

Lemma 3.3 $\mathcal{A}_{\mathrm{sa}} \subseteq \Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}] + \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}}$.

Proof Consider the set of formal words in $2n$ symbols $x_1, \ldots, x_n, (1+x_1^2)^{-1}, \ldots, (1+x_n^2)^{-1}$ that do not contain subwords $x_j(1+x_j^2)^{-1}$ or $(1+x_j^2)^{-1}x_j^2$; it maps injectively into $\mathcal{A}$, and its image, denoted $\mathcal{E}$, is a basis of $\mathcal{A}$. An expansion of $a \in \mathcal{A}$ with respect to $\mathcal{E}$ will be called *the normal form* of a. That is, univariate sub-expressions in a are written as partial fractions, with the inverses on the left for the sake of bookkeeping.

It suffices to show that $u + u^* \in \Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}] + \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}}$ for all $u \in \mathcal{E}$. This is done by consecutively eliminating $(1+x_1^2)^{-1}, \ldots, (1+x_n^2)^{-1}$ from u; we demonstrate this only for $(1+x_1^2)^{-1}$, and the other $(1+x_j^2)^{-1}$ are eliminated in the same manner.

Every $v \in \mathcal{E}$ can be uniquely written as

$$v = v_0(1+x_1^2)^{-m_1}v_1(1+x_1^2)^{-m_2}v_2\cdots(1+x_1^2)^{-m_\ell}v_\ell$$

where $m_k > 0$ and $v_k \in \mathcal{E}$ with $v_j \neq 1$ for $0 < j < \ell$ do not contain $(1 + x_1^2)^{-1}$. Set $\delta(v) = \ell$. More generally, for $a \in \mathcal{A}$ let $\delta(a)$ be the maximum of $\delta(v)$ for v appearing in the normal form of a.

Assume that $(1 + x_1^2)^{-1}$ appears in u (as otherwise there is nothing to be done); that is, $\delta(u) \geq 1$. After subtracting an element of $[\mathcal{A}, \mathcal{A}]$ from $u + u^*$ and taking a maximal term with respect to δ, we can assume that u starts with $(1 + x_1^2)^{-1}$. We can write $u = u'(1 + x_1^2)^{-m}u''$ for $m > 0$ and $u', u'' \in \mathcal{E}$ with $\delta(u') = \lfloor \frac{\delta(u)}{2} \rfloor$ and $\delta(u'') = \delta(u) - 1 - \delta(u')$. Then

$$\begin{aligned} u + u^* = {} & \big(u' + u''^*\big)(1 + x_1^2)^{-m}\big(u' + u''^*\big)^* \\ & + u'(1 - (1 + x_1^2)^{-m})u'^* \\ & + u''^*(1 - (1 + x_1^2)^{-m})u'' \\ & - u'u'^* - u''^*u''. \end{aligned} \tag{3.2}$$

The first three terms of (3.2) belong to $\Sigma^2\mathcal{A}$ by Lemma 3.1(e). Furthermore, note that $\delta(u''u''^*) < \delta(u)$, and since u' is either 1 (if $\delta(u) = 1$) or starts with $(1 + x_1^2)^{-1}$, there is $c \in [\mathcal{A}, \mathcal{A}]$ such that $\delta(u'u'^* - c) < \delta(u)$. Using (3.2) and induction on $\delta(u)$ it then follows that $u + u^* \in \Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}] + \mathbb{R}<\underline{x}>_{\mathrm{sa}}$. □

Let $\mathcal{A}_{\mathbb{C}} = \mathbb{C} \otimes_{\mathbb{R}} \mathcal{A}$ denote the complexification of $\mathcal{A}$.

Lemma 3.4 *Every linear functional $\varphi : \mathbb{R}<\underline{x}>_{\mathrm{sa}} \to \mathbb{R}$ satisfying $\varphi(\mathcal{K}) = \mathbb{R}_{\geq 0}$ extends to a linear $*$-functional $\phi : \mathcal{A}_{\mathbb{C}} \to \mathbb{C}$ satisfying $\phi(\Sigma^2\mathcal{A}_{\mathbb{C}} + [\mathcal{A}_{\mathbb{C}}, \mathcal{A}_{\mathbb{C}}]) = \mathbb{R}_{\geq 0}$.*

Proof Note that $\Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}]$ is a convex cone in $\mathcal{A}_{\mathrm{sa}}$, and

$$\mathcal{A}_{\mathrm{sa}} = \Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}] \cap \mathcal{A}_{\mathrm{sa}} + \mathbb{R}<\underline{x}>_{\mathrm{sa}}$$

by Lemma 3.3. Hence φ extends to a linear fuctional $\phi' : \mathcal{A}_{\mathrm{sa}} \to \mathbb{R}$ that satisfies $\phi'(\Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}] \cap \mathcal{A}_{\mathrm{sa}}) = \mathbb{R}_{\geq 0}$ by the Riesz extension theorem [53, Proposition 1.7]. Let $\rho, \iota : \mathcal{A}_{\mathbb{C}} \to \mathcal{A}$ be $\mathbb{R}$-linear maps given by $\rho(a) = \frac{1}{2}(a + \overline{a})$ and $\iota(a) = \frac{1}{2i}(a - \overline{a})$. Thus $a = \rho(a) + i\iota(a)$ for $a \in \mathcal{A}_{\mathbb{C}}$. Let $\phi : \mathcal{A}_{\mathbb{C}} \to \mathbb{C}$ be defined as

$$\phi(a) = \frac{1}{2}\phi'(\rho(a) + \rho(a)^*) + \frac{i}{2}\phi'(\iota(a) + \iota(a)^*)$$

for $a \in \mathcal{A}_{\mathbb{C}}$. Then ϕ is a $*$-functional,

$$\phi([a, b]) = \phi\Big([\rho(a), \rho(b)] - [\iota(a), \iota(b)] + i\big([\rho(a), \iota(b)] + [\iota(a), \rho(b)]\big)\Big) = 0$$

and

$$\begin{aligned} \phi(aa^*) &= \phi\Big(\rho(a)\rho(a)^* + \iota(a)\iota(a)^* + i\big(\iota(a)\rho(a)^* - \rho(a)\iota(a)^*\big)\Big) \\ &= \phi'\big(\rho(a)\rho(a)^* + \iota(a)\iota(a)^*\big) \geq 0 \end{aligned}$$

for all $a, b \in \mathcal{A}_{\mathbb{C}}$. Therefore $\phi(\Sigma^2\mathcal{A}_{\mathbb{C}} + [\mathcal{A}_{\mathbb{C}}, \mathcal{A}_{\mathbb{C}}]) = \mathbb{R}_{\geq 0}$. □

4 Unbounded tracial moment problem

The tracial analog of the moment problem for probability measures with compact support was solved in [19, 45]. To obtain our rational Positivstellensatz on global trace positivity, one has to consider analogs of probability measures with non-compact support. In this section we solve the unbounded tracial moment problem for noncommutative joint distributions.

Proposition 4.1 *For every linear $*$-functional $\phi : \mathcal{A}_{\mathbb{C}} \to \mathbb{C}$ satisfying $\phi(1) = 1$ and $\phi(\Sigma^2\mathcal{A}_{\mathbb{C}} + [\mathcal{A}_{\mathbb{C}}, \mathcal{A}_{\mathbb{C}}]) = \mathbb{R}_{\geq 0}$ there exist a tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in L^{\omega}(\mathcal{F}, \tau)^n_{\mathrm{sa}}$ such that $\phi(a) = \tau(a(\underline{X}))$ for all $a \in \mathcal{A}_{\mathbb{C}}$.*

Proof We split the proof, which is a version of the Gelfand–Naimark–Segal construction for unbounded functionals on $\mathcal{A}$ that produces power-integrable operators, in several steps.

Step 1: Construction of unbounded operators. On $\mathcal{A}_{\mathbb{C}}$ we define a semi-scalar product $\langle a, b\rangle = \phi(ab^*)$. By the Cauchy–Schwarz inequality for semi-scalar products,

$$\mathcal{N} = \{a \in \mathcal{A}_{\mathbb{C}} \colon \phi(aa^*) = 0\}$$

is a vector subspace of $\mathcal{A}_{\mathbb{C}}$ and $\mathcal{N}^* = \mathcal{N}$. Furthermore, for every $a \in \mathcal{N}$, $b \in \mathcal{A}_{\mathbb{C}}$ and $\varepsilon > 0$ we have

$$0 \leq \phi\left((a^* \pm \varepsilon b)(a^* \pm \varepsilon b)^*\right) = \varepsilon\left(\varepsilon\phi(bb^*) \pm 2\,\mathrm{Re}\,\phi(ba)\right);$$

since $\varepsilon > 0$ was arbitrary, and a can be replaced by ia, it follows that $ba, ab \in \mathcal{N}$. Hence $\mathcal{N}$ is an ideal in $\mathcal{A}_{\mathbb{C}}$. Let $\mathcal{H}$ be the completion of $\mathcal{A}_{\mathbb{C}}/\mathcal{N}$ with respect to $\langle\cdot,\cdot\rangle$. Then $\mathcal{H}$ is a separable Hilbert space; let $\vec{a} \in \mathcal{H}$ denote the vector corresponding to $a \in \mathcal{A}_{\mathbb{C}}$. The left multiplication by x_j in $\mathcal{A}_{\mathbb{C}}$ induces a densely defined symmetric operator X'_j on $\mathcal{H}$. In particular, X'_j is closable by [52, Section 3.1]; let X_j be its closure. Since $x_j^2 + 1$ is invertible in $\mathcal{A}$, the elements $x_j + i$ and $x_j - i$ in $\mathcal{A}_{\mathbb{C}}$ are also invertible. Hence the linear operators $X'_j + iI$ and $X'_j - iI$ are invertible on $\mathcal{A}_{\mathbb{C}}/\mathcal{N}$. Therefore X_j is a self-adjoint operator by [52, Proposition 3.8]. Note that

$$a(\underline{X})\vec{b} = \overrightarrow{ab}$$

for all $a, b \in \mathcal{A}_{\mathbb{C}}$. Then $-i$ belongs to the resolvent set of X_j, the resolvent $(X_j + iI)^{-1}$ is a bounded operator on $\mathcal{H}$ and

$$\mathrm{ran}(X_j + iI)^{-1} = \mathrm{dom}\, X_j \tag{4.1}$$

by [52, Proposition 3.10].

Step 2: A tracial von Neumann algebra. Let $\mathcal{F} \subseteq \mathcal{B}(\mathcal{H})$ be the von Neumann algebra generated by $(X_1 + iI)^{-1}, \ldots, (X_n + iI)^{-1}$, i.e., the weak operator topology closure of the unital $*$-algebra generated by $(X_1 + iI)^{-1}, \ldots, (X_n + iI)^{-1}$. Define $\tau : \mathcal{F} \to \mathbb{C}$ as $\tau(F) = \langle F\vec{1}, \vec{1}\rangle$. Then τ is a faithful normal state on $\mathcal{F}$. Furthermore,

τ is tracial. Indeed, let P, Q be arbitrary elements of the unital $*$-algebra generated by $(X_1+iI)^{-1},\ldots,(X_n+iI)^{-1}$. Then $P=p(\underline{X})$ and $Q=q(\underline{X})$ for some $p,q\in\mathcal{A}_{\mathbb{C}}$. Since $\phi([\mathcal{A}_{\mathbb{C}},\mathcal{A}_{\mathbb{C}}])=\{0\}$, we have

$$\tau(PQ)=\phi(pq)=\phi(qp)=\tau(QP).$$

By construction, the Hilbert space $L^2(\mathcal{F},\tau)$ naturally embeds into $\mathcal{H}$. In fact, $L^2(\mathcal{F},\tau)=\mathcal{H}$. To see this, it suffices to show that $\overrightarrow{a}\in L^2(\mathcal{F},\tau)$ implies $\overrightarrow{x_ja}\in L^2(\mathcal{F},\tau)$ for every $a\in\mathcal{A}$ and $j=1,\ldots,n$. Suppose $\overrightarrow{a}\in L^2(\mathcal{F},\tau)$; let $K\subset\mathcal{H}$ be the closure of $\{\overrightarrow{pa}\colon p\in\mathbb{C}[x_j,(1+x_j^2)^{-1}]\}$, and let $K_0\subseteq L^2(\mathcal{F},\tau)$ be the image of $\overrightarrow{a}$ under the $*$-algebra generated by $(X_j+iI)^{-1}$. Note that $(x_j\pm i)^{-1}\in\mathbb{C}[x_j,(1+x_j^2)^{-1}]$. The map

$$\mathbb{C}\left[t,\tfrac{1}{t\pm i}\right]\to K,\qquad f\mapsto\overrightarrow{f(x_j)a}$$

induces a Hilbert space isomorphism

$$L^2(\mathbb{R},\mu)\to K \tag{4.2}$$

where μ is the finite measure on $\mathbb{R}$ satisfying

$$\int_{\mathbb{R}} f\,\mathrm{d}\mu=\phi(f(x_j)aa^*)$$

for $f\in\mathbb{C}[t,\frac{1}{t\pm i}]$. The preimage of K_0 under the isomorphism (4.2) contains the set $\{(t\pm i)^{-k}\colon k\in\mathbb{N}_0\}$. Therefore K_0 is dense in K by [53, Lemma 6.9]. Thus in particular $\overrightarrow{x_ja}\in K=\overline{K_0}\subset L^2(\mathcal{F},\tau)$, as desired.

Step 3: Affiliation. Let $U\in\mathcal{B}(\mathcal{H})$ be a unitary in the commutant of $\mathcal{F}$. Since

$$U(X_j+iI)^{-1}=(X_j+iI)^{-1}U \tag{4.3}$$

and $\operatorname{ran}(X_j+iI)^{-1}=\operatorname{dom}X_j$ by (4.1), we have $U\operatorname{dom}X_j\subseteq\operatorname{dom}X_j$. Moreover, (4.3) then implies

$$(X_j+iI)U(X_j+iI)^{-1}(X_j+iI)=(X_j+iI)(X_j+iI)^{-1}U(X_j+iI)$$

on $\operatorname{dom}X_j$, from where we conclude $X_jU=UX_j$ on $\operatorname{dom}X_j$. Since the unitary U in the commutant of $\mathcal{F}$ was arbitrary, the self-adjoint operator X_j on $\mathcal{H}$ is affiliated with $\mathcal{F}$.

Step 4: Integrability. Since the positive semidefinite operator X_j^2 is affiliated with $\mathcal{F}$, by the spectral theorem there exists a projection valued measure E_λ with values in $\mathcal{F}$ such that $X_j^2=\int_0^\infty\lambda\,\mathrm{d}E_\lambda$. Then for every $p\in\mathbb{N}$,

$$\tau(|X_j|^{2p})=\tau(X_j^{2p})=\int_0^\infty\lambda^p\,\mathrm{d}\tau(E_\lambda)=\int_0^\infty\lambda^p\,\mathrm{d}\langle E_\lambda\overrightarrow{1},\overrightarrow{1}\rangle=\langle X_j^{2p}\overrightarrow{1},\overrightarrow{1}\rangle<\infty,$$

where the second equality holds by [38, Section 3], the third equality holds by the definition of integration, and the inequality holds since $\vec{1} \in \operatorname{dom} X_j^{2p}$. Therefore $X_j \in L^{2p}(\mathcal{F}, \tau)$. As $p \in \mathbb{N}$ was arbitrary, it follows that $X_j \in L^{\omega}(\mathcal{F}, \tau)$.

Step 5: Conclusion. Finally, we have

$$\tau(a(\underline{X})) = \langle a(\underline{X})\vec{1}, \vec{1}\rangle = \phi(a)$$

for every $a \in \mathcal{A}_{\mathbb{C}}$. □

Let $(\mathcal{F}, \tau)$ be a tracial von Neumann algebra and $\underline{X} \in L^{\omega}(\mathcal{F}, \tau)^n_{\mathrm{sa}}$. The functional $p \mapsto \tau(p(\underline{X}))$ on $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ is called a *noncommutative joint distribution* (cf. [57, Section 2.3] or [37, Section 6.4]). We obtain the following tracial version of Haviland's theorem [35, Theorem 3.1.2].

Theorem 4.2 *Let $\varphi : \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \to \mathbb{R}$ be a linear functional with $\varphi(1) = 1$. Then φ is a noncommutative joint distributionif and only if $\varphi(\mathcal{K}) = \mathbb{R}_{\geq 0}$.*

Proof ($\Rightarrow$) is straightforward. ($\Leftarrow$) The functional φ extends to a $*$-functional $\phi : \mathcal{A}_{\mathbb{C}} \to \mathbb{C}$ satisfying $\phi(\Sigma^2 \mathcal{A}_{\mathbb{C}} + [\mathcal{A}_{\mathbb{C}}, \mathcal{A}_{\mathbb{C}}]) \geq 0$ by Lemma 3.4. Then $\varphi(p) = \phi(p) = \tau(p(\underline{X}))$ for some $(\mathcal{F}, \tau)$ and $\underline{X} \in L^{\omega}(\mathcal{F}, \tau)^n_{\mathrm{sa}}$, and all $p \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$, by Proposition 4.1. □

Remark 4.3 The cone $\Sigma^2\mathbb{R}\langle \underline{x} \rangle + [\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle]$ is closed in $\mathbb{R}\langle \underline{x} \rangle$ by [6, Proposition 1.58 and Corollary 3.11] and [53, Remark A.29] and does not contain $\mathcal{K}$ by Lemma 3.1(d). The condition "$\varphi \geq 0$ on $\mathcal{K}$" is therefore more restrictive than "$\varphi \geq 0$ on $\Sigma^2\mathbb{R}\langle \underline{x} \rangle + [\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle]$".

The proof of Proposition 4.1 actually implies a more general version of Theorem 4.2. Let $S \subset \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$. Denote

$$\mathcal{K}_S := \left([\mathcal{A}, \mathcal{A}] + \sum_{s \in \{1\} \cup S} s \cdot \Sigma^2 \mathcal{A} \right) \cap \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}. \tag{4.4}$$

In particular, $\mathcal{K}_{\emptyset}$ equals $\mathcal{K}$ from (3.1). Let us say that the functional $p \mapsto \tau(p(\underline{X}))$ for some tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in L^{\omega}(\mathcal{F}, \tau)^n_{\mathrm{sa}}$ is noncommutative joint distributionconstrained by S if $s(\underline{X}) \geq 0$ for all $s \in S$.

Corollary 4.4 *Let $\varphi : \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \to \mathbb{R}$ be a linear functional with $\varphi(1) = 1$. Then φ is a noncommutative joint distributionconstrained by $S \subset \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ if and only if $\varphi(\mathcal{K}_S) = \mathbb{R}_{\geq 0}$.*

Proof ($\Rightarrow$) is again straightforward. For ($\Leftarrow$), recall the construction of $(\mathcal{F}, \tau)$ and $\underline{X} \in L^{\omega}(\mathcal{F}, \tau)^n$ from the proof of Proposition 4.1. Then for every $s \in S$ and $a \in \mathcal{A}_{\mathbb{C}}$,

$$\langle s(\underline{X})\mathbf{a}, \mathbf{a}\rangle = \varphi(saa^*) \geq 0.$$

Therefore $\tau(s(\underline{X})FF^*) \geq 0$ for every $F \in \mathcal{F}$, whence $s(\underline{X}) \succeq 0$. □

5 A commutative intermezzo and bivariate trace-positive polynomials

In this section, we give a commutative analog of Theorem 4.2, and establish a refined solution of Hilbert's 17th problem for commutative bivariate polynomials that lifts to a positivity certificate for a special class of nc polynomials.

Let $\underline{t} = (t_1, \ldots, t_n)$ be commuting indeterminates, and consider the convex cone

$$\mathcal{C} = \mathbb{R}[\underline{t}] \cap \Sigma^2\mathbb{R}\left[t_1, \ldots, t_n, \tfrac{1}{1+t_1^2}, \ldots, \tfrac{1}{1+t_n^2}\right]$$

in $\mathbb{R}[\underline{t}]$. We start by recording the commutative counterpart of Theorem 4.2. While it follows from [53, Theorem 13.33 and Example 13.36] and it can be proved in a similar way as Proposition 4.1 (with adaptations regarding strongly commuting operators as in [43, Corollary 2.6]), we provide a simpler independent argument, inspired by real algebraic geometry.

Proposition 5.1 *Let $\varphi : \mathbb{R}[\underline{t}] \to \mathbb{R}$ be a linear functional with $\varphi(1) = 1$. Then φ comes from a probability measure if and only if $\varphi(\mathcal{C}) = \mathbb{R}_{\geq 0}$.*

Proof Only the backward implication is nontrivial. Let $h = (1 + t_1^2) \cdots (1 + t_n^2)$, and $A = \mathbb{R}[\underline{t}, \frac{1}{h}]$. By a variant of Schmüdgen's Positivstellensatz [35, Corollary 3.5.2], every bounded nonnegative $f \in A$ lies in the closure (with respect to the finest locally convex topology) of $\Sigma^2 A$ in A. On the other hand, every $f \in A$ becomes bounded when divided by a sufficiently high power of h. Therefore, the closure of $\Sigma^2 A$ agrees with the convex cone of nonnegative functions in A. The rest follows by Haviland's theorem [35, Theorem 3.1.2]. □

Next, we give a new strenghened solution of Hilbert's 17th problem for bivariate polynomials.

Theorem 5.2 *If $f \in \mathbb{R}[t_1, t_2]$ is nonnegative on $\mathbb{R}^2$ then there exists $k \in \mathbb{N}$ such that $(1 + t_1^2)^k f$ is a sum of squares in $\mathbb{R}[t_1, t_2]$.*

Proof We wish to show that f is a sum of squares in the ring of fractions

$$A = \mathbb{R}[t_1, t_2]_{1+t_1^2} = \left\{(1 + t_1^2)^{-k} p \colon p \in \mathbb{R}[t_1, t_2],\ k \in \mathbb{N}_0\right\}.$$

The ring A is the coordinate ring of the affine real variety $X = Y \times \mathbb{A}^1$, where Y is the projective line $\mathbb{P}^1$ minus one real point $[0 : 1]$ and two complex conjugate nonreal points $[1 : \pm i]$. Let $S \subset \mathbb{A}^2$ be the plane affine curve $t_1^2 + t_2^2 = 1$. Then S is isomorphic to $\mathbb{P}^1$ minus two complex conjugate points $[1 : \pm i]$. So $Y \cong S\backslash\{x\}$ where x is a real point of S, and hence $X \cong (S \times \mathbb{A}^1)\backslash L$ is isomorphic to $S \times \mathbb{A}^1$ minus the real line $L = \{x\} \times \mathbb{A}^1$. Let $q \in \mathbb{R}[S]$ be such that x is the only (real or complex) zero of q in S. Then $A = \mathbb{R}[X]$ is isomorphic to ring of fractions $\mathbb{R}[S \times \mathbb{A}^1]_q = \{q^{-k} g \colon g \in \mathbb{R}[S \times \mathbb{A}^1], k \in \mathbb{N}_0\}$. To show that every nonnegative polynomial function on X is a sum of squares in A, it therefore suffices to see that every nonnegative polynomial

function on $S \times \mathbb{A}^1$ is a sum of squares in $\mathbb{R}[S \times \mathbb{A}^1]$. The latter is in fact true and was proved in [51, Theorem 2]. □

Remark 5.3 Recall that every nonnegative real polynomial is a sum of squares of rational functions (by Hilbert's 17th problem, as solved by Artin). Speaking informally, Theorem 5.2 states that $1 + t_1^2$ is a uniform denominator for such sums of squares in the case of two variables. Let us point out how this relates to several previous results. If $h \in \mathbb{R}[t_1, t_2]$ is such that its homogenization is a positive definite form, then for every nonnegative $f \in \mathbb{R}[t_1, t_2]$ there exists $k \in \mathbb{N}$ such that $h^k f$ is a sum of squares in $\mathbb{R}[t_1, t_2]$ ([48, Corollary 3.12]). This result applies, in particular, to $h = 1 + t_1^2 + t_2^2$, but not to $h = 1 + t_1^2$. In fact, one checks easily that Theorem 5.2 implies the statement for $h = 1 + t_1^2 + t_2^2$.

A weaker uniform denominator result, which however is valid for any number of variables, says that if the homogenizations of f, $h \in \mathbb{R}[t_1, \ldots, t_n]$ are both positive definite, then there exists $k \in \mathbb{N}$ such that $h^k f$ is a sum of squares of polynomials ([46] for $h = 1 + \sum_i t_i^2$ and [50, Remark 4.6] in general).

Let us now apply the preceding commutative result to a special class of bivariate nc polynomials. Let $n = 2$ and $\underline{x} = (x_1, x_2)$. We say that $f \in \mathbb{R}\langle x_1, x_2\rangle$ is **cyclically sorted** [28, Definition 4.1] if

$$f \in \operatorname{span}\{x_1^i x_2^j : i, j \in \mathbb{N}_0\} + [\mathbb{R}\langle x_1, x_2\rangle, \mathbb{R}\langle x_1, x_2\rangle].$$

The noncommutative lift of the Motzkin polynomial in Example 3.2 is cyclically sorted.

Corollary 5.4 *If $f \in \mathbb{R}\langle x_1, x_2\rangle_{\mathrm{sa}}$ is cyclically sorted, then the following are equivalent:*

(i) $f(\underline{\xi}) \geq 0$ *for all* $\underline{\xi} \in \mathbb{R}^2$;
(ii) $\tau(f(\underline{X})) \geq 0$ *for all* $\underline{X} \in \mathrm{M}_k(\mathbb{C})^2_{\mathrm{sa}}$ *and* $k \in \mathbb{N}$;
(iii) $\tau(f(\underline{X})) \geq 0$ *for every tracial von Neumann algebra* $(\mathcal{F}, \tau)$ *and* $\underline{X} \in \mathcal{F}^2_{\mathrm{sa}}$;
(iv) $f \in \mathcal{K}$.

Proof (iv)⇒(iii)⇒(ii)⇒(i) is clear.

(i)⇒(iv) Let $\pi : \mathbb{R}\langle x_1, x_2, (1+x_1^2)^{-1}\rangle \to \mathbb{R}[t_1, t_2, (1+t_1^2)^{-1}]$ be the homomorphism given by $\pi(x_1) = t_1$ and $\pi(x_2) = t_2$. Let

$$V = \operatorname{span}\{(1 + x_1^2)^{-k} x_1^i x_2^j : i, j, k \in \mathbb{N}_0\} \subset \mathbb{R}\langle x_1, x_2, (1 + x_1^2)^{-1}\rangle$$

and observe that there is a unique linear map $\eta : \mathbb{R}[t_1, t_2, (1 + t_1^2)^{-1}] \to V$ such that $\pi \circ \eta = \mathrm{id}$. Furthermore,

$$\begin{aligned}\eta\Big((1+t_1^2)^{-k_1} t_1^{i_1} t_2^{j_1}\Big)\eta\Big((1+t_1^2)^{-k_2} t_1^{i_2} t_2^{j_2}\Big)^* &= (1+x_1^2)^{-k_1} x_1^{i_1} x_2^{j_1+j_2} x_1^{i_2} (1+x_1^2)^{-k_2} \\ &= (1+x_1^2)^{-k_1-k_2} x_1^{i_1+i_2} x_2^{j_1+j_2} \\ &\quad + \Big[(1+x_1^2)^{-k_1} x_1^{i_1} x_2^{j_1+j_2}, x_1^{i_2}(1+x_1^2)^{-k_2}\Big]\end{aligned}$$

and so

$$\eta(a)\eta(b)^* \in V + [\mathcal{A}, \mathcal{A}] \tag{5.1}$$

for all $a, b \in \mathbb{R}[t_1, t_2, (1+t_1^2)^{-1}]$. By (i), $\pi(f)$ is a nonnegative bivariate polynomial, so by Theorem 5.2 there exist $s_1, \ldots, s_\ell \in \mathbb{R}[t_1, t_2, (1+t_1^2)^{-1}]$ such that $\pi(f) = s_1^2 + \cdots + s_\ell^2$. Then

$$\tilde{f} := \eta(s_1)\eta(s_1)^* + \cdots + \eta(s_\ell)\eta(s_\ell)^* \in \mathcal{K}.$$

Since $f, \tilde{f} \in V + [\mathcal{A}, \mathcal{A}]$ by (5.1) and $\pi(f) = \pi(\tilde{f})$, we have $f - \tilde{f} \in [\mathcal{A}, \mathcal{A}]$. Therefore $f \in \mathcal{K}$. □

6 Globally trace-positive polynomials

In this section we characterize multivariate trace-positive polynomials as the closure of $\mathcal{K}$ in Theorem 6.1. Closedeness and stability of the cone $\mathcal{K}$ are also discussed. Furthermore, Proposition 6.4 touches upon a connection between global trace positivity and Connes' embedding problem.

6.1 A Positivstellensatz

Solvability of the general moment problem gives rise to the following description of trace-positive polynomials.

Theorem 6.1 *For $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$, the following are equivalent:*

(i) $\tau(f(\underline{X})) \geq 0$ *for every tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in \mathcal{F}_{\mathrm{sa}}^n$;*
(ii) $\tau(f(\underline{X})) \geq 0$ *for every tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in L^\omega(\mathcal{F}, \tau)_{\mathrm{sa}}^n$;*
(iii) $\tau(f(\underline{X})) \geq 0$ *for every tracial von Neumann algebra $(\mathcal{F}, \tau)$ and $\underline{X} \in L^{\deg f}(\mathcal{F}, \tau)_{\mathrm{sa}}^n$;*
(iv) *f lies in the closure of $\mathcal{K}$ with respect to the finest locally convex topology on $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$.*

Proof (iii)⇒(ii)⇒(i) Clear.

(i)⇒(iii) Let $p = \deg f$. Suppose $\tau(f(\underline{X})) < 0$ for some $\underline{X} \in L^p(\mathcal{F}, \tau)_{\mathrm{sa}}^n$. By Hölder's inequality (2.1) and the triangle inequality, there exists a positive constant c such that for every $Y \in L^p(\mathcal{F}, \tau)$ satisfying $\|X_1 - Y\|_p \leq 1$,

$$\left|\tau(f(X_1, \ldots, X_n)) - \tau(f(Y, X_2, \ldots, X_n))\right| \leq c\|X_1 - Y\|_p. \tag{6.1}$$

By [55, Theorem IX.2.13(ii)], $\mathcal{F}$ is dense in $L^p(\mathcal{F}, \tau)$ with respect to the p-norm. Hence by (6.1) there exists $Y_1 \in \mathcal{F}$ such that $\tau(f(Y_1, X_2, \ldots, X_n)) < 0$. Continuing in this fashion, we can replace each X_j with a bounded operator Y_j, and thus obtain $\underline{Y} \in \mathcal{F}^n$ that satisfies $\tau(f(\underline{Y})) < 0$.

(ii)⇒(iv) By the Hahn-Banach separation theorem [2, Theorem 3.4], $f \notin \overline{\mathcal{K}}$ if and only if there is a functional $\varphi : \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \to \mathbb{R}$ such that $\varphi(f) < 0$ and $\varphi(\mathcal{K}) = \mathbb{R}_{\geq 0}$.

Note that such a functional is nonzero, and $\varphi(p)^2 \leq \varphi(1)\varphi(p^2)$ for all $p \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ implies $\varphi(1) > 0$; thus we can rescale it to $\varphi(1) = 1$. By Theorem 4.2, there exist $(\mathcal{F}, \tau)$ and $\underline{X} \in L^\omega(\mathcal{F}, \tau)^n_{\mathrm{sa}}$ such that $\varphi(p) = \tau(p(\underline{X}))$ for $p \in \mathbb{R}\langle \underline{x} \rangle$. Then $\tau(f(\underline{X})) < 0$.

(iv)$\Rightarrow$(ii) Every $\underline{X} \in L^\omega(\mathcal{F}, \tau)^n_{\mathrm{sa}}$ gives rise to a functional $\phi : a \mapsto \tau(a(\underline{X}))$ on $\mathcal{A}$, and $\phi(\mathcal{K}) = \mathbb{R}_{\geq 0}$. The restriction of ϕ to $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ is continuous with respect to the finest locally convex topology on $\mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$. Hence $f \in \overline{\mathcal{K}}$ implies $\phi(f) \geq 0$. □

Remark 6.2 In Theorem 6.1, it suffices to restrict to II_1 factors $\mathcal{F}$ (which have unique tracial states), since every tracial von Neumann algebra embeds into a II_1 factor [13, Theorem 2.5] (cf. [25, Proposition 2.2]).

For $R > 0$ let

$$\mathcal{M}_R = \Sigma^2\mathbb{R}\langle \underline{x} \rangle + [\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle] + \sum_{j=1}^{n} (R - x_j^2) \cdot \Sigma^2\mathbb{R}\langle \underline{x} \rangle \,.$$

We can also describe the closure of $\mathcal{K}$ without denominators as follows (another alternative with fewer quantifiers is given in Theorem 7.2 below).

Corollary 6.3 *The closure of $\mathcal{K}$ in the finest locally convex topology equals*

$$\overline{\mathcal{K}} = \left\{ f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \colon f + \varepsilon \in \mathcal{M}_R \text{ for all } \varepsilon, R > 0 \right\}. \tag{6.2}$$

Proof By Theorem 6.1, $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ belongs to $\overline{\mathcal{K}}$ if and only if it has nonnegative trace on all tuples of operators from tracial von Neumann algebras. In other words, for every $R > 0$ we have $\tau(f(\underline{X})) \geq 0$ for all $\underline{X} \in \mathcal{F}^n$ with $\|X_1\|, \ldots, \|X_n\| \leq \sqrt{R}$. By [28, Theorem 3.12], such f belongs to the right-hand side of (6.2). □

6.2 Trace positivity on matrices

Theorem 6.1 considers global trace positivity over all tracial von Neumann algebras, which in principle could coincide with global trace positivity over matrices of all finite dimensions. The recent resolution of Connes' embedding problem [23] is equivalent to the existence of:

(1) an everywhere convergent nc power series that has nonnegative trace on all matrix tuples, but not on a tuple of operators from a von Neumann algebra [45, Corollary 1.2];
(2) an nc polynomial that has nonnegative trace on all tuples of matrix contractions, but not on a tuple of contractions from a von Neumann algebra [28, Theorem 1.6].

In the context of global trace positivity of nc polynomials, these facts inspire the following (superficially stronger) statement.

Proposition 6.4 *There exists $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ such that*

(i) $\mathrm{tr}(f(\underline{X})) \geq 0$ *for all $\underline{X} \in \mathrm{M}_k(\mathbb{C})^n_{\mathrm{sa}}$ and $k \in \mathbb{N}$;*

(ii) $\tau(f(\underline{Y})) < 0$ *for some tracial von Neumann algebra* $(\mathcal{F}, \tau)$ *and* $\underline{Y} \in \mathcal{F}_{\mathrm{sa}}^n$.

To prove this, we first relate trace positivity on arbitrary matrix tuples with the existence of matricial microstates in free probability [56].

Proposition 6.5 *For a tracial von Neumann algebra* $(\mathcal{F}, \tau)$ *and* $\underline{Y} \in \mathcal{F}_{\mathrm{sa}}^n$, *the following are equivalent:*

(i) *for every* $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$, $\mathrm{tr}(f(\underline{X})) \geq 0$ *for all* $\underline{X} \in \mathrm{M}_k(\mathbb{C})_{\mathrm{sa}}^n$ *and* $k \in \mathbb{N}$ *implies* $\tau(f(\underline{Y})) \geq 0$;
(ii) *for all* $\varepsilon > 0$ *and* $d \in \mathbb{N}$ *there are* $k \in \mathbb{N}$ *and* $\underline{X} \in \mathrm{M}_k(\mathbb{C})_{\mathrm{sa}}^n$ *such that*

$$\left| \tau(w(\underline{Y})) - \frac{1}{k} \mathrm{tr}(w(\underline{X})) \right| < \varepsilon$$

for all $w \in \langle \underline{x} \rangle_d$.

Proof The implication (ii)⇒(i) clearly holds.

Now assume (i) holds, and fix $d \in \mathbb{N}$. Let $L \in \mathbb{R}\langle \underline{x} \rangle_d^{\vee}$ be given by $L(p) = \mathrm{Re}\, \tau(p(\underline{Y}))$, and let $C \subseteq \mathbb{R}\langle \underline{x} \rangle_d^{\vee}$ be the closed convex hull of

$$C_0 = \left\{ p \mapsto \frac{1}{k} \mathrm{Re}\, \mathrm{tr}(p(\underline{X})) \colon k \in \mathbb{N}, \underline{X} \in \mathrm{M}_k(\mathbb{C})^n \right\}.$$

Suppose $L \notin C$. By the Hahn-Banach separation theorem, there exist $f_0 \in \mathbb{R}\langle \underline{x} \rangle_d \cong \mathbb{R}\langle \underline{x} \rangle_d^{\vee\vee}$ and $\gamma \in \mathbb{R}$ such that $L(f_0) < \gamma < L'(f_0)$ for all $L' \in C$. Let $f = \frac{1}{2}(f + f^*) - \gamma \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$. Then $L(f) < 0 < L'(f)$ for all $L' \in C_0$, which contradicts (i).

Therefore (i) implies $L \in C$, so every neighborhood of L in $\mathbb{R}\langle \underline{x} \rangle_d^{\vee}$ contains a convex combination with rational coefficients of elements in C_0. By arranging finite sets of matrices into block diagonal matrices, we see that C_0 is closed under convex combinations with rational coefficients. Thus every neighborhood of L contains an element of C_0, so (ii) holds. □

Proof of Proposition 6.4 Combine Proposition 6.5, the equivalence of Connes' embedding problem and existence of microstates [10, Proposition 3.3] (also e.g. [56, Section 7.4] or [40, Theorem 7]), and the resolution of Connes' embedding problem [23, Section 1.3]. □

6.3 The cone $\mathcal{K}$ is neither closed nor stable

In this subsection we explore further properties of the cone $\mathcal{K}$. We require two auxiliary lemmas.

Lemma 6.6 *Let* $a_0, a_1, a_2 \geq 0$ *and* $n \in \mathbb{N}$. *If* $a_2 a_0^n \geq n^n a_1^{n+1}$ *then* $a_2 - (n+1)a_1 + a_0 \geq 0$.

Proof If $a_0 = 0$, then $a_1 = 0$, and so $a_2 - (n+1)a_1 + a_0 \geq 0$ holds. If $a_0 \neq 0$, then

$$\begin{aligned} a_2 - (n+1)a_1 + a_0 &\geq \frac{n^n a_1^{n+1}}{a_0^n} - (n+1)a_1 + a_0 \\ &= \frac{a_0}{n}\left(\left(\frac{na_1}{a_0}\right)^{n+1} - (n+1)\left(\frac{na_1}{a_0}\right) + n\right) \\ &= \frac{a_0}{n}\left(\frac{na_1}{a_0} - 1\right)\sum_{k=0}^{n-1}\left(\left(\frac{na_1}{a_0}\right)^k - 1\right). \end{aligned}$$

The last two factors are both nonnegative if $na_1 \geq a_0$ and both negative if $na_1 < a_0$, so $a_2 - (n+1)a_1 + a_0 \geq 0$ holds. □

Lemma 6.7 *Let $(\mathcal{F}, \tau)$ be a tracial von Neumann algebra and let $a, b \in \mathcal{F}_{\mathrm{sa}}$. Then*

$$2\tau\left((ba^2b)^{\frac{3}{2}}\right) \leq \tau\left(a^4b^2 + b^2a^4\right).$$

Proof By the Araki–Lieb–Thirring inequality [34] (more precisely, its von Neumann algebra version [30, Corollary 3]),

$$\tau\left((ba^2b)^{\frac{3}{2}}\right) = \tau\left((|b||a|^2|b|)^{\frac{3}{2}}\right) \leq \tau\left(|b|^{\frac{3}{2}}|a|^3|b|^{\frac{3}{2}}\right) = \tau\left(|a|^3|b|^3\right).$$

Then

$$\begin{aligned} \tau\left(a^4b^2 + a^2b^4\right) - 2\tau\left((ba^2b)^{\frac{3}{2}}\right) &\geq \tau\left(|a|^2|b|^2|a|^2 + |a||b|^4|a|\right) - 2\tau\left(|a|^3|b|^3\right) \\ &= \tau\left((|a|^2|b| - |a||b|^2)(|b||a|^2 - |b|^2|a|)\right) \end{aligned}$$

is nonnegative. □

A witness of $\mathcal{K} \neq \overline{\mathcal{K}}$ for $n \geq 3$ is a noncommutative lift of the homogenized Motzkin polynomial.

Proposition 6.8 *Let*

$$h = x_2^2x_1^2x_2^2 + x_1^2x_2^2x_1^2 + x_3^6 - 3x_1x_2x_3^2x_2x_1 \in \mathbb{R}\langle \underline{x} \rangle.$$

Then $h \in \overline{\mathcal{K}} \backslash \mathcal{K}$.

Proof Consider the commutative homogenized Motzkin polynomial

$$H = t_1^4t_2^2 + t_1^2t_2^4 - 3t_1^2t_2^2t_3^2 + t_3^6 \in \mathbb{R}[t_1, t_2, t_3]$$

which is not a sum of squares in $\mathbb{R}[t_1, t_2, t_3]$ by [35, Proposition 1.2.4]. If $h \in \mathcal{K}$, then $(1 + t_1^2)^{k_1}(1 + t_2^2)^{k_2}(1 + t_3^2)^{k_3}H$ is a sum of squares in $\mathbb{R}[t_1, t_2, t_3]$ for some

$k_1, k_2, k_3 \in \mathbb{N}$. The lowest-degree homogeneous part of a sum of squares is again a sum of squares, so H is a sum of squares in $\mathbb{R}[t_1, t_2, t_3]$, a contradiction. Therefore $h \notin \mathcal{K}$.

Next we prove $h \in \overline{\mathcal{K}}$. Let $(\mathcal{F}, \tau)$ be a tracial von Neumann algebra, and $X_1, X_2, X_3 \in \mathcal{F}_{\mathrm{sa}}$. Set

$$a_0 = \tau(X_1^4 X_2^2 + X_1^2 X_2^4), \quad a_1 = \tau(X_2 X_1^2 X_2 X_3^2), \quad a_2 = \tau(X_3^6).$$

Note that $a_0, a_1, a_2 \geq 0$. By Hölder's inequality (2.1) (with $p_1 = \frac{3}{2}$ and $p_2 = 3$),

$$4\Big(\tau(X_2 X_1^2 X_2 X_3^2)\Big)^3 \leq 4\Big(\tau\left((X_2 X_1^2 X_2)^{\frac{3}{2}}\right)\Big)^2 \tau(X_3^6) \leq \Big(\tau\left(X_1^4 X_2^2 + X_1^2 X_2^4\right)\Big)^2 \tau(X_3^6).$$

Therefore $4a_1^3 \leq a_2 a_0^2$. Hence

$$\tau(h(X_1, X_2, X_3)) = a_0 - 3a_1 + a_2 \geq 0$$

by Lemma 6.6. Since $(\mathcal{F}, \tau)$ and X_1, X_2, X_3 were arbitrary, $h \in \overline{\mathcal{K}}$ by Theorem 6.1. □

Remark 6.9 Consider $\mathcal{A}$ with the finest locally convex topology. That is, every linear functional on $\mathcal{A}$ is continuous. Then $[\mathcal{A}, \mathcal{A}]$ is a closed subspace, and $\Sigma^2\mathcal{A}$ is a closed convex cone in $\mathcal{A}$ by [26, Theorem 4.5]. On the other hand, if $n \geq 3$ then $\Sigma^2\mathcal{A} + [\mathcal{A}, \mathcal{A}]$ is not closed by Proposition 6.8.

A desired property of a convex cone generated by (hermitian) squares is stability [35, Section 4.1]. Let us adapt this notion to our context. We say that $a \in \mathcal{A}$ is of *degree at most d* if a can be written as an nc polynomial of degree at most d in the generators of $\mathcal{A}$. The cone $\mathcal{K}$ is *stable* if there exists a function $\Delta\colon \mathbb{N} \to \mathbb{N}$ such that for every $d \in \mathbb{N}$ and $f \in \mathcal{K}$ of degree at most d, there are $s_1, \ldots, s_\ell \in \mathcal{A}$ of degree at most $\Delta(d)$ such that $f - s_1 s_1^* - \cdots - s_\ell s_\ell^* \in [\mathcal{A}, \mathcal{A}]$.

Lemma 6.10 *If $n \geq 2$ then $\mathcal{K}$ is not stable.*

Proof Suppose $\mathcal{K}$ is stable. Let $M = t_1^4 t_2^2 + t_1^2 t_2^4 - 3t_1^2 t_2^2 + 1 \in \mathbb{R}[t_1, t_2]$ be the Motzkin polynomial, and let $m = x_2 x_1^4 x_2 + x_2^2 x_1^2 x_2^2 - 3x_2 x_1^2 x_2 + 1 \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ be its noncommutative lift as in Example 3.2. For $\lambda \in \mathbb{R}$ denote $M_\lambda(t_1, t_2) = M(\lambda t_1, \lambda t_2) \in \mathbb{R}[t_1, t_2]$ and $m_\lambda(x_1, x_2) = m(\lambda x_1, \lambda x_2) \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$. By Corollary 5.4, $m_\lambda \in \mathcal{K}$ for all λ. Note that m_λ is of degree at most 6 for every λ. Thus by the stability assumption there exists $d' \in \mathbb{N}$ such that for every λ there are $s_k \in \mathcal{A}$ of degree at most d' such that $m_\lambda - \sum_k s_k s_k^* \in [\mathcal{A}, \mathcal{A}]$. Consequently $(1+t_1^2)^{d'}(1+t_2^2)^{d'} M_\lambda$ is a sum of squares of polynomials in $\mathbb{R}[t_1, t_2]$ for every λ. But this is impossible by the proof of [47, Theorem 1]. Indeed, if $\lambda \neq 0$ and the polynomial $(1 + t_1^2)^{d'}(1 + t_2^2)^{d'} M_\lambda$ of degree $4d' + 6$ is a sum of squares, then so is $(1 + \frac{1}{\lambda^2} t_1^2)^{d'}(1 + \frac{1}{\lambda^2} t_2^2)^{d'} M$. Since the cone of sums of squares of degree at most $4d' + 6$ is closed [33, Corollary 3.34], taking the limit $\lambda \to \infty$ implies that M is a sum of squares in $\mathbb{R}[t_1, t_2]$, a contradiction. □

Remark 6.11 It is unclear whether $\overline{\mathcal{K}}$ coincides with the sequential closure $\mathcal{K}^{\ddagger}$ of $\mathcal{K}$ [8],

$$\mathcal{K}^{\ddagger} = \{f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} : \text{there is } g \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}} \text{ such that } f + \varepsilon g \in \mathcal{K} \text{ for every } \varepsilon > 0\}.$$

See Theorem 7.2 below for a description of $\overline{\mathcal{K}}$ resembling $\mathcal{K}^{\dagger}$.

Remark 6.12 Membership in $\mathcal{K}$ can be certified with a sequence of semidefinite programs. Namely, $f \in \mathbb{R}\langle \underline{x} \rangle_{\mathrm{sa}}$ belongs to $\mathcal{K}$ if and only if

$$f = \sum_i s_i s_i^* + \sum_j [a_j, b_j], \qquad s_j, a_j, b_j \in \mathcal{A}_d \tag{6.3}$$

for some $d \in \mathbb{N}$, and (6.3) can be rephrased as a feasibility semidefinite program. Similarly, for $d \in \mathbb{N}$ let μ_d be the solution of the optimization problem

$$\begin{aligned} \inf_{\substack{L:\mathcal{A}_{2d}\to\mathbb{R} \\ L \text{linear}}} \quad & L(f) \\ s.t. \quad & L(1) = 1\,, \\ & L(ab) = L(ba)\,, \quad \text{for all } a, b \in \mathcal{A}_d\,, \\ & L(s^*s) \geq 0\,, \quad \text{for all } s \in \mathcal{A}_{2d}\,. \end{aligned} \tag{6.4}$$

Then (6.4) is a semidefinite program, and $(\mu_d)_d$ is an increasing sequence of lower bounds for $\inf_{(\mathcal{F},\tau),\underline{X}\in\mathcal{F}^n} \tau(f(\underline{X}))$.

6.4 Tracial arithmetic-geometric mean inequality

The following tracial version of the renowned arithmetic-geometric mean inequality is essentially known, and can be deduced from the generalized Hölder's inequality for unitarily invariant norms [5, Exercise IV.2.7] (cf. [14, Theorem 4.2]) applied to the nuclear norm on a tracial von Neumann algebra. We present an alternative argument inspired by the proof of Proposition 6.8.

Proposition 6.13 *Let $(\mathcal{F}, \tau)$ be a tracial von Neumann algebra. Then*

$$\frac{\tau(f_1 + \cdots + f_n)}{n} \geq \tau\left(\left(\left(f_1^{\frac{1}{2}} \cdots f_n^{\frac{1}{2}}\right)^* \left(f_1^{\frac{1}{2}} \cdots f_n^{\frac{1}{2}}\right)\right)^{\frac{1}{n}}\right) \tag{6.5}$$

for all positive semidefinite $f_1, \ldots, f_n \in \mathcal{F}$.

Proof We prove (6.5) by induction on n. If $n = 1$, (6.5) is an equality. Now assume (6.5) holds for n. Let $f_1, \ldots, f_{n+1} \succeq 0$, and set $f = f_n^{\frac{1}{2}} \cdots f_1^{\frac{1}{2}} f_1^{\frac{1}{2}} \cdots f_n^{\frac{1}{2}}$. By the

Araki-Lieb-Thirring inequality [30, Corollary 3] and Hölder's inequality (2.1) with $p_1 = n+1$ and $p_2 = \frac{n+1}{n}$,

$$\begin{aligned}\tau\left(\left(f_{n+1}^{\frac{1}{2}} f f_{n+1}^{\frac{1}{2}}\right)^{\frac{1}{n+1}}\right) &\le \tau\left(f_{n+1}^{\frac{1}{2(n+1)}} f^{\frac{1}{n+1}} f_{n+1}^{\frac{1}{2(n+1)}}\right)\\ &= \tau\left(f_{n+1}^{\frac{1}{n+1}} f^{\frac{1}{n+1}}\right)\\ &\le \tau\left(f_{n+1}\right)^{\frac{1}{n+1}} \cdot \tau\left(f^{\frac{1}{n}}\right)^{\frac{n}{n+1}}.\end{aligned}$$

Therefore

$$n^n \tau\left(\left(f_{n+1}^{\frac{1}{2}} f f_{n+1}^{\frac{1}{2}}\right)^{\frac{1}{n+1}}\right)^{n+1} \le \tau\left(f_{n+1}\right) \cdot \left(n\tau\left(f^{\frac{1}{n}}\right)\right)^n. \tag{6.6}$$

By the induction hypothesis,

$$n\,\tau\left(f^{\frac{1}{n}}\right) \le \tau\left(f_1 + \cdots + f_n\right). \tag{6.7}$$

Let

$$\begin{aligned}a_0 &= \tau\left(f_1 + \cdots + f_n\right),\\ a_1 &= \tau\left(\left(f_{n+1}^{\frac{1}{2}} \cdots f_1^{\frac{1}{2}} f_1^{\frac{1}{2}} \cdots f_{n+1}^{\frac{1}{2}}\right)^{\frac{1}{n+1}}\right),\\ a_2 &= \tau\left(f_{n+1}\right).\end{aligned}$$

Then (6.6) and (6.7) imply $n^n a_1^{n+1} \le a_2 a_0^n$, so $a_2 + a_0 - (n+1)a_1 \ge 0$ by Lemma 6.6. Therefore (6.5) holds for $n+1$. □

Remark 6.14 Other (weaker) inequalities resembling (6.5) are

$$\frac{\tau(f_1 + \cdots + f_n)}{n} \ge \left|\tau\left(f_1^{\frac{1}{n}} \cdots f_n^{\frac{1}{n}}\right)\right|, \tag{6.8}$$

which holds by (2.1) and the classical algebraic-geometric mean inequality, and

$$\frac{\sqrt{\tau(f_1^2)} + \cdots + \sqrt{\tau(f_n^2)})}{n} \ge \sqrt{\tau\left(\left(\left(f_1^{\frac{1}{2}} \cdots f_n^{\frac{1}{2}}\right)^* \left(f_1^{\frac{1}{2}} \cdots f_n^{\frac{1}{2}}\right)\right)^{\frac{2}{n}}\right)} \tag{6.9}$$

which follows by [5, Exercise IV.2.7] applied to the Hilbert-Schmidt norm on $(\mathcal{F}, \tau)$.

7 Denominator-free characterization of global trace positivity

While Section 6 gives an algebraic certificate for trace positivity in terms of sums of hermitian squares with denominators, this section presents an alternative that involves only nc polynomials. First, we give a sufficient condition for solvability of the unbounded tracial moment problem (Theorem 7.1). Next, we show that every trace-positive nc polynomial can be perturbed to a sum of hermitian squares and commutators of nc polynomials (Theorem 7.2). Finally, we demonstrate this principle explicitly on (a noncommutative lift of) the Motzkin polynomial.

7.1 Tracial Carleman's condition

In this subsection we show that a variant of Carleman's condition for the Hamburger moment problem [53, Corollary 4.10] is a sufficient condition for a functional to be a noncommutative joint distribution. The following is a tracial version of Nussbaum's theorem [53, Theorem 14.19].

Theorem 7.1 *Let $\varphi : \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}} \to \mathbb{R}$ be a linear functional satisfying $\varphi(1) = 1$ and $\varphi(pp^*) = \varphi(p^*p) \geq 0$ for all $p \in \mathbb{R}\langle \underline{x}\rangle$. If there is $M > 0$ such that*

$$\varphi(x_j^{2r}) \leq (2r)!M^r \qquad \text{for all } r \in \mathbb{N} \text{ and } j = 1, \ldots, n, \tag{7.1}$$

then φ is a noncommutative joint distribution.

Proof We extend φ to a $*$-functional $\phi : \mathbb{C}\langle \underline{x}\rangle \to \mathbb{C}$ as

$$\phi(p) = \frac{1}{4}\varphi(p + p^* + \overline{p} + \overline{p}^*) + \frac{i}{4}\varphi(-ip + ip^* + i\overline{p} - i\overline{p}^*)$$

for $p \in \mathbb{R}\langle \underline{x}\rangle$. As in the proof of Lemma 3.4 we see that $\phi(pp^*) = \phi(p^*p) \geq 0$ for $p \in \mathbb{C}\langle \underline{x}\rangle$, and then

$$\phi([p, q]) = \frac{1}{2}\phi([p, q] + [q^*, p^*]) = \frac{1}{2}\phi\Big((p - q^*)^*(p - q^*) - (p - q^*)(p - q^*)^*\Big) = 0$$

for $p, q \in \mathbb{C}\langle \underline{x}\rangle$. Therefore $\phi(\Sigma^2\mathbb{C}\langle \underline{x}\rangle) = \mathbb{R}_{\geq 0}$ and $\phi([\mathbb{C}\langle \underline{x}\rangle, \mathbb{C}\langle \underline{x}\rangle]) = \{0\}$. We proceed with another variation of the Gelfand–Naimark–Segal construction following the same steps as in the proof of Proposition 4.1.

Step 1: Construction of unbounded operators. On $\mathbb{C}\langle \underline{x}\rangle$, there is a semi-scalar product $\langle p, q\rangle = \phi(pq^*)$. As in Step 1 of the proof of Proposition 4.1, it gives rise to a separable Hilbert space $\mathcal{H}$. Let $\mathcal{D} = \{\vec{p} \in \mathcal{H} \colon p \in \mathbb{C}\langle \underline{x}\rangle\}$, which is a dense subspace of $\mathcal{H}$. For $j = 1, \ldots, n$ let X'_j be symmetric operators on $\mathcal{D}$ induced by left multiplication by x_j on $\mathbb{C}\langle \underline{x}\rangle$. Let $\widetilde{X}_j$ be the closure of X'_j. Note that $\mathcal{D} \subseteq \operatorname{dom} w(\widetilde{\underline{X}})$ for every $w \in \langle \underline{x}\rangle$.

Set $R = \frac{1}{5\sqrt{M}} > 0$, and fix $1 \leq j \leq n$. Let $p \in \mathbb{C}\langle \underline{x} \rangle$ and $t \in (-R, R)$ be arbitrary. By the triangle inequality and the Cauchy–Schwarz inequality,

$$\begin{aligned}\left\| \sum_{k=m}^{\infty} \frac{(it)^k}{k!} \widetilde{X}_j^k \vec{p} \right\| &\leq \sum_{k=m}^{\infty} \frac{|t|^k}{k!} \left\| \widetilde{X}_j^k \vec{p} \right\| \\ &= \sum_{k=m}^{\infty} \frac{|t|^k}{k!} \sqrt{\phi(x_j^{2k} pp^*)} \\ &\leq \sum_{k=m}^{\infty} \frac{|t|^k}{k!} \sqrt[4]{\phi(x_j^{4k})} \sqrt[4]{\phi((pp^*)^2)} \\ &\leq \sqrt[4]{\phi((pp^*)^2)} \sum_{k=m}^{\infty} (\sqrt{M}|t|)^k \frac{\sqrt[4]{(4k)!}}{k!}\end{aligned} \tag{7.2}$$

is arbitrary small for large $m \in \mathbb{N}$ since the series

$$\sum_{k=0}^{\infty} \frac{\sqrt[4]{(4k)!}}{k! \cdot 5^k}$$

is absolutely convergent by the ratio test. Therefore for every $t \in (-R, R)$ there is a well-defined linear map $\widetilde{U}_j(t) : \mathcal{D} \to \mathcal{H}$,

$$\widetilde{U}_j(t) = \exp\left(it\widetilde{X}_j\right) = \sum_{k=0}^{\infty} \frac{(it)^k}{k!} \widetilde{X}_j^k.$$

By the properties of the exponential function we see that $\widetilde{U}_j(t)$ is an isometry, and thus uniquely extends to an isometry $U_j(t) : \mathcal{H} \to \mathcal{H}$. Furthermore, $U_j(t)^* = U_j(-t)$ and $U_j(-t)U_j(t) = U_j(t)U_j(-t) = I$ on $\mathcal{D}$, and therefore on $\mathcal{H}$, so $U_j(t)$ is a unitary. Furthermore, $U_j(s)U_j(t) = U_j(s+t)$ for all $s, t, s+t \in (-R, R)$. Therefore we can extend the family $\{U_j(t) : t \in (-R, R)\}$ to a well-defined one-parametric unitary group $\{U_j(t) : t \in \mathbb{R}\}$, uniquely determined by

$$U_j(ma) = U_j(a)^m \tag{7.3}$$

for all $a \in (-R, R)$ and $m \in \mathbb{Z}$. Furthermore, this one-parametric group is strongly continuous by (7.2) and (7.3). By Stone's theorem [52, Theorem 6.2] there is a unique self-adjoint operator X_j on $\mathcal{H}$ such that $U_j(t) = \exp(itX_j)$ for all $t \in \mathbb{R}$, and

$$\begin{aligned}\operatorname{dom} X_j &= \left\{ v \in \mathcal{H} \colon \lim_{\varepsilon \to 0} \frac{1}{\varepsilon}\big(U_j(\varepsilon)v - v\big) \text{ exists} \right\}, \\ X_j v &= \lim_{\varepsilon \to 0} \frac{-i}{\varepsilon}\big(U_j(\varepsilon)v - v\big) \qquad \text{for all } v \in \operatorname{dom} X_j\end{aligned} \tag{7.4}$$

by [52, Proposition 5.1]. In particular, for $\vec{p} \in \mathcal{D}$ we have $X_j \vec{p} = \widetilde{X}_j \vec{p}$ by the definition of $\widetilde{U}_j(t)$ and $U_j(t)$, so X_j is an extension of $\widetilde{X}_j$.

Step 2: A tracial von Neumann algebra. Let $\mathcal{F} \subseteq \mathcal{B}(\mathcal{H})$ be the von Neumann algebra generated by $U_j(t)$ for $j = 1, \ldots, n$ and $t \in \mathbb{R}$. Define $\tau : \mathcal{F} \to \mathbb{C}$ as $\tau(F) = \langle F\vec{1}, \vec{1}\rangle$. Note that

$$\langle p(\widetilde{\underline{X}})q(\widetilde{\underline{X}})\vec{1}, \vec{1}\rangle = \phi(pq) = \phi(qp) = \langle q(\widetilde{\underline{X}})p(\widetilde{\underline{X}})\vec{1}, \vec{1}\rangle$$

for all $p, q \in \mathbb{R}\langle \underline{x}\rangle$. By estimating as in (7.2) we see that

$$\begin{aligned}
\langle w_1(\widetilde{\underline{U}})w_2(\widetilde{\underline{U}})\vec{1}, \vec{1}\rangle &= \lim_{m\to\infty} \left\langle w_1\left(\sum_{k=0}^{m} \frac{(it)^k}{k!}\widetilde{\underline{X}}^k\right) w_2\left(\sum_{k=0}^{m} \frac{(it)^k}{k!}\widetilde{\underline{X}}^k\right)\vec{1}, \vec{1}\right\rangle \\
&= \lim_{m\to\infty} \left\langle w_2\left(\sum_{k=0}^{m} \frac{(it)^k}{k!}\widetilde{\underline{X}}^k\right) w_1\left(\sum_{k=0}^{m} \frac{(it)^k}{k!}\widetilde{\underline{X}}^k\right)\vec{1}, \vec{1}\right\rangle \\
&= \langle w_2(\widetilde{\underline{U}})w_1(\widetilde{\underline{U}})\vec{1}, \vec{1}\rangle
\end{aligned}$$

for all $w_1, w_2 \in \langle \underline{x}\rangle$. Therefore

$$\tau(w_1(\underline{U})w_2(\underline{U})) = \tau(w_2(\underline{U})w_1(\underline{U}))$$

for all $w_1, w_2 \in \langle \underline{x}\rangle$, so τ is a faithful normal tracial state on $\mathcal{F}$. By construction, the Hilbert space $L^2(\mathcal{F}, \tau)$ naturally embeds into $\mathcal{H}$. Since $\mathcal{D} = \operatorname{span}\{w(\underline{X})\vec{1} : w \in \langle \underline{x}\rangle\}$, we have $\mathcal{D} \subset L^2(\mathcal{F}, \tau)$ by (7.4). Therefore $\mathcal{H} = L^2(\mathcal{F}, \tau)$.

Step 3: Affiliation. Let $V \in \mathcal{B}(\mathcal{H})$ be a unitary in the commutant of $\mathcal{F}$, and fix $1 \le j \le n$. Then V commutes with all $U_j(t)$. If $v \in \operatorname{dom} X_j$, then $\frac{1}{\varepsilon}(U_j(\varepsilon)v - v)$ converges as $\varepsilon \to 0$. Then the same holds for

$$V \cdot \frac{1}{\varepsilon}(U_j(\varepsilon)v - v) = \frac{1}{\varepsilon}(U_j(\varepsilon)Vv - Vv),$$

so $Vv \in \operatorname{dom} X_j$, and $VX_jv = X_jVv$ by (7.4). Thus V commutes with X_j. Consequently the self-adjoint operators $X_1, \ldots, X_n$ are affiliated with $\mathcal{F}$.

Step 4: Integrability. Follows exactly as in Step 4 of the proof of Proposition 4.1.

Step 5: Conclusion. By construction we have

$$\tau(p(\underline{X})) = \langle p(\underline{X})\vec{1}, \vec{1}\rangle = \phi(p)$$

for every $p \in \mathbb{C}\langle \underline{x}\rangle$. □

7.2 Approximation with sums of hermitian squares and commutators

The aim of this subsection is to establish the tracial version of Lasserre's perturbation result [31, 32] for globally positive polynomials.

Theorem 7.2 *For $f \in \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}}$, the following are equivalent:*

(i) $\tau(f(\underline{X})) \geq 0$ *for every tracial von Neumann algebra* $(\mathcal{F}, \tau)$ *and* $\underline{X} \in \mathcal{F}_{\mathrm{sa}}^n$;
(ii) *for each* $\varepsilon > 0$ *there exists* $r \in \mathbb{N}$ *such that*

$$f + \varepsilon \sum_{j=1}^{n} \sum_{k=0}^{r} \frac{1}{k!} x_j^{2k} \in \Sigma^2\mathbb{R}\langle \underline{x}\rangle + [\mathbb{R}\langle \underline{x}\rangle, \mathbb{R}\langle \underline{x}\rangle].$$

For $r \in \mathbb{N}$ denote

$$\Omega_r = \sum_{j=1}^{n} \sum_{k=0}^{r} \frac{1}{k!} x_j^{2k}.$$

Note that $\Omega_r - n \in \Sigma^2\mathbb{R}\langle \underline{x}\rangle$. Two optimization problems will be key in the proof of Theorem 7.2. Let $r \in \mathbb{N}$ and $M \in \mathbb{R}_{>0}$, and consider

$$Q_{r,M}: \begin{cases} \inf\limits_{\substack{L:\mathbb{R}\langle \underline{x}\rangle_{2r} \to \mathbb{R} \\ L \text{ linear, self-adjoint, tracial}}} & L(f) \\ s.t. & L(M - \Omega_r) \geq 0\,, \\ & L(1) = 1\,, \\ & L(p^*p) \geq 0 \quad \text{for all } p \in \mathbb{R}\langle \underline{x}\rangle_r\,; \end{cases} \tag{7.5}$$

$$Q_{r,M}^{\vee}: \begin{cases} \sup\limits_{z \in \mathbb{R}} & z \\ s.t. & f - z \in \Theta_{2r}^2 + \mathbb{R}_{\geq 0}(M - \Omega_r)\,. \end{cases} \tag{7.6}$$

Here $\Theta_{2r}^2 \subset \mathbb{R}\langle \underline{x}\rangle_{\mathrm{sa}}$ is the set of all (symmetric) nc polynomials of degree $\leq 2r$ that are cyclically equivalent to sums of (degree $\leq r$) squares. Recall [28]: two words $u, v \in \langle \underline{x}\rangle$ are called cyclically equivalent ($u \overset{\mathrm{cyc}^*}{\sim} v$) if v or v^* can be obtained from u by cyclically rotating the letters in u. For notational convenience, let $\mathcal{C}_{r,M} = \Theta_{2r}^2 + \mathbb{R}_{\geq 0}(M - \Omega_r)$.

Lemma 7.3 *The optimization problems (7.5) and (7.6) are semidefinite programs dual to each other.*

Proof This is a variation on what is now standard material, cf. [6]. Encode the tracial linear functional $L : \mathbb{R}\langle \underline{x}\rangle_{2r} \to \mathbb{R}$ with its Hankel matrix $\mathbf{M}(L)_{u,v} = L(u^*v)$ for $u, v \in \langle \underline{x}\rangle_r$. With this (7.5) can be rewritten as

$$Q_{r,M}: \begin{cases} \inf & \langle \mathbf{M}(L),\, \mathbf{G}(f)\rangle \\ s.t. & \Big\langle \mathbf{M}(L),\, \mathbf{G}(M - \Omega_r)\Big\rangle \geq 0\,, \\ & \mathbf{M}(L)_{u,v} = \mathbf{M}(L)_{\hat{u},\hat{v}} \quad \text{if } u^*v \overset{\mathrm{cyc}^*}{\sim} \hat{u}^*\hat{v}\,, \\ & \mathbf{M}(L)_{1,1} = 1\,, \\ & \mathbf{M}(L) \succeq 0\,. \end{cases} \tag{7.7}$$

where $\mathbf{G}(f)$ denote a Gram matrix of f, i.e., $f = \mathbb{V}_r^* \mathbf{G}(f) \mathbb{V}_r$ if $\mathbb{V}_r$ denote the vector of all words in $\underline{x}$ of degree $\leq r$. Now (7.7) is easily seen to be a SDP: the objective function is linear in the entries of $\mathbf{M}(L)$, the first constraint is a linear inequality on the entries of $\mathbf{M}(L)$, the equality constraints give rise to a finite set of linear equations on the entries of $\mathbf{M}(L)$, and the last constraint is a positivity constraint on $\mathbf{M}(L)$.

To recognize that (7.6) is an SDP, observe that $f - z \in \mathcal{C}_{r,M}$ if and only if there is a Gram matrix $\mathbf{G}(f)$, a positive semidefinite $G \succeq 0$ and $\lambda \geq 0$ such that

$$\mathbb{V}_r^* \mathbf{G}(f) \mathbb{V}_r - z \overset{\text{cyc}^*}{\sim} \mathbb{V}_r^* G \mathbb{V}_r + \lambda(M - \Omega_r). \tag{7.8}$$

Clearly, (7.8) yields linear constraints on the entries of G, so maximizing z over the set of feasible G is a semidefinite program.

We shall now use a standard Lagrange duality approach to show the SDPs (7.5) and (7.6) are dual to each other:

$$\begin{aligned}
\sup_{f-z \in \mathcal{C}_{r,M}} z &= \sup_z \inf_{L \in \mathcal{C}_{r,M}^\vee} (z + L(f - z)) \\
&\leq \inf_{L \in \mathcal{C}_{r,M}^\vee} \sup_z (z + L(f - z)) \\
&= \inf_{L \in \mathcal{C}_{r,M}^\vee} \big(L(f) + \sup_z z(1 - L(1)) \big) \\
&= \inf \big\{ L(f) \mid L \in \mathcal{C}_{r,M}^\vee,\ L(1) = 1 \big\}.
\end{aligned}$$

The first equality comes from the fact that the inner minimization problem gives minimal value 0 if and only if $f - z \in \mathcal{C}_{r,M}$. The inequality in this chain is obvious. The inner maximization problem in the next to last line is bounded with maximum value 0 if and only $L(1) = 1$. Finally, the optimization problem on the last line is equivalent to (7.5). □

Lemma 7.4 *The convex cone $\mathcal{C}_{r,M}$ is closed in the finite dimensional Euclidean space $\mathbb{R}<\underline{x}>_{2r}$.*

Proof The cone Θ_{2r}^2 is well-known to be closed [6, Proposition 1.58]. Hence the conclusion follows from [4, Theorem 3.2]. □

Lemma 7.5 *Strong duality holds for the pair of SDPs (7.5) and (7.6).*

Proof Let $\inf Q_{r,M}$ denote the optimal value of (7.5) and let $\sup Q_{r,M}^\vee$ denote the optimal value of (7.6). By Lemma 7.3 and weak duality from semidefinite programming [2, Theorem IV.6.2], $\sup Q_{r,M}^\vee \leq \inf Q_{r,M}$. If $M < n$, then (7.5) is not feasible, and $\sup Q_{r,M}^\vee = \infty$ because $\mathcal{C}_{r,M} = \mathbb{R}<\underline{x}>_{2r}$. Hence let $M \geq n$. Then $\mathbf{M}(L) = E_{11}$ is clearly feasible for (7.5), whence $\inf Q_{r,M} < \infty$.

Suppose that (7.6) is feasible, $-\infty < \sup Q_{r,M}^\vee \leq \inf Q_{r,M}$. Note that $L(f - \inf Q_{r,M}) \geq 0$ for all $L \in \mathcal{C}_{r,M}^\vee$. This implies that $f - \inf Q_{r,M}$ is in $\mathcal{C}_{r,M}^{\vee\vee} = \mathcal{C}_{r,M}$ since $\mathcal{C}_{r,M}$ is closed by Lemma 7.4. Hence $\sup Q_{r,M}^\vee \geq \inf Q_{r,M}$.

Finally, suppose that (7.6) is infeasible. Then for every $\lambda \in \mathbb{R}$, $f - \lambda \notin \mathcal{C}_{r,M}$. By the Hahn-Banach separation theorem [2, Theorem III.1.3], there exists a linear functional

$L \in \mathcal{C}_{r,M}^{\vee}$ with $L(\mathcal{C}_{r,M}) \subseteq \mathbb{R}_{\geq 0}$, $L(1) = 1$ and $L(f) < \lambda$. As λ was arbitrary, this shows (7.5) is unbounded, establishing strong duality. □

Lemma 7.6 *Suppose $f \in \mathbb{R}\langle \underline{x} \rangle$ is uniformly bounded below on tracial von Neumann algebras, in the sense that $f_\star := \inf_{(\mathcal{F},\tau),\underline{X}\in\mathcal{F}^n} \tau(f(\underline{X})) > -\infty$. Then (7.5) is feasible for $2r \geq \deg f$ and $M \geq n$, and $\inf Q_{r,M} \nearrow f_M$ as $r \to \infty$ for some $f_M \geq f_\star$.*

Proof Feasibility of (7.5) for $2r \geq \deg f$ and $M \geq n$ is clear (e.g., $L(p) = p(0)$ for $p \in \mathbb{R}\langle \underline{x} \rangle_{2r}$). If L is feasible for $Q_{r,M}$ then its restriction is feasible for $Q_{r',M}$ for $r' < r$. Hence the sequence $(\inf Q_{r,M})_{r\geq d}$ is increasing.

Let L be feasible for $Q_{r,M}$. Observe that for $k \leq r$, the values of $L(x_j^{2k})$ are bounded by the linear inequality,

$$L(x_j^{2k}) \leq k!M. \tag{7.9}$$

Then Hadwin's noncommutative Hölder inequality for linear functionals on the free algebra (see [19, Proof of Theorem 1.3]) implies a bound

$$|L(x_{i_1} \cdots x_{i_\delta})| \leq \prod_{j=1}^{\delta} \sqrt[2^\delta]{L(x_{i_j}^{2^\delta})} \leq \prod_{j=1}^{\delta} \sqrt[2^\delta]{(2^{\delta-1})!M} =: c_\delta$$

for all $2^\delta \leq 2r$. In particular, if $r \geq 2^{\deg f - 1}$ then $L(f) \leq s \cdot c_{\deg f}$, where s is the number of summands in f.

Hence $(\inf Q_{r,M})_r$ is an increasing function bounded from above, whence $\inf Q_{r,M} \nearrow f_M$ as $r \to \infty$, for some f_M. It remains to show $f_M \geq f_\star$.

To each $L : \mathbb{R}\langle \underline{x} \rangle \to \mathbb{R}$ we assign the infinite Hankel matrix $\mathbf{M}(L)$ as in the proof of Lemma 7.3. If L acts only on $\mathbb{R}\langle \underline{x} \rangle_{2r}$ we extend it by 0 to all of $\mathbb{R}\langle \underline{x} \rangle$. We also scale each $L : \mathbb{R}\langle \underline{x} \rangle \to \mathbb{R}$ to $\check{L} : \mathbb{R}\langle \underline{x} \rangle \to \mathbb{R}$ by $\check{L}(w) = \frac{1}{c_{|w|}} L(w)$ for a word $w \in \langle \underline{x} \rangle$.

Let $L^{(r)}$ be an optimizer of (7.5), and consider the sequence $(\mathbf{M}(\check{L}^{(r)}))_{r\in\mathbb{N}}$. Each entry in each infinite matrix is bounded by 1 in absolute value, so we may consider this a sequence in the unit ball B_1 of ℓ^∞. By the Banach-Alaoglu theorem [2, Theorem III.2.9], B_1 is compact in the weak-$*$ topology of ℓ^∞. Hence there is an element $\mathbf{M} = \mathbf{M}(\check{L})$ in B_1 and a subsequence $(\mathbf{M}(\check{L}^{(r_k)}))_{k\in\mathbb{N}}$ converging to $\mathbf{M}(\check{L})$. In particular, $\check{L}^{(r_k)}(w) \to \check{L}(w)$ as $k \to \infty$, for all $w \in \langle \underline{x} \rangle$. Now define

$$\hat{L} : \mathbb{R}\langle \underline{x} \rangle \to \mathbb{R}, \quad w \mapsto c_{|w|}\check{L}(w).$$

Then $L^{(r_k)}|_{\mathbb{R}\langle \underline{x} \rangle_\delta} \to \hat{L}|_{\mathbb{R}\langle \underline{x} \rangle_\delta}$ as $k \to \infty$, for every $\delta \in \mathbb{N}$. In particular, $\hat{L}$ is a $*$-functional, $\hat{L}(1) = 1$, $\hat{L}(f) = f_M$, $\hat{L}([\mathbb{R}\langle \underline{x} \rangle, \mathbb{R}\langle \underline{x} \rangle]) = \{0\}$ and $\hat{L}(\Sigma^2\mathbb{R}\langle \underline{x} \rangle) = \mathbb{R}_{\geq 0}$.

Let $m \in \mathbb{N}$ be arbitrary. Then for every $r_k \geq m$,

$$L^{(r_k)}(x_j^{2m}) \leq m!M$$

by (7.9). Consequently

$$\hat{L}(x_j^{2m}) \leq m!M.$$

Therefore L is a noncommutative joint distributionby Theorem 7.1. In particular, $f_M \geq f_\star$ since $f_\star = \inf_{(\mathcal{F},\tau),\underline{X}\in L^\omega(\mathcal{F},\tau)^n} \tau(f(\underline{X}))$ by (i)⇔(ii) of Theorem 6.1. □

Proof of Theorem 7.2 (ii)⇒(i) Let $(\mathcal{F},\tau)$ and $\underline{X} \in \mathcal{F}_{\rm sa}^n$ be arbitrary. Then for every $r \in \mathbb{N}$,

$$\tau\left(\Omega_r(\underline{X})\right) \leq \sum_{j=1}^n \tau\left(\exp(X_j^2)\right) =: M < \infty.$$

By (ii), for every $\varepsilon > 0$ there exists $r \in \mathbb{N}$ such that

$$\tau\left(f(\underline{X}) + \varepsilon\Omega_r(\underline{X})\right) \geq 0.$$

Therefore for every $\varepsilon > 0$,

$$\tau(f(\underline{X})) \geq -\varepsilon M,$$

and so $\tau(f(\underline{X})) \geq 0$.

(i)⇒(ii) Denote $f_\star = \inf_{(\mathcal{F},\tau),\underline{X}} \tau(f(\underline{X}))$.

First assume $f_\star > 0$. Let $M > \max\{\frac{1}{f_\star}, n\}$ be arbitrary. By Lemmas 7.5 and 7.6 there exists $r_M > 0$ such that $\sup Q^\vee_{r_M,M} > f_\star - \frac{1}{M}$. That is, there are $z_M \geq f_\star - \frac{1}{M}$, $\lambda_M \geq 0$ and $q_M \in \Theta^2_{2r_M}$ such that

$$f - z_M = q_M + \lambda_M\left(M - \Omega_{r_M}\right). \tag{7.10}$$

Evaluating (7.10) at $\underline{X} = 0 \in \mathbb{R}^n$ gives

$$f(0) - f_\star + \frac{1}{M} \geq f(0) - z_M = q_M(0) + \lambda_M(M - \Omega_{r_M}(0)) \geq \lambda_M(M-n),$$

and therefore

$$\lambda_M \leq \frac{f(0) - f_\star + \frac{1}{M}}{M-n}. \tag{7.11}$$

The right-hand side of (7.11) goes to 0 as $M \to \infty$. By (7.10),

$$f + \lambda_M\Omega_{r_M} = z_M + q_M + \lambda_M M \in \Theta^2_{2r_M},$$

and $\lambda_M \to 0$ as $M \to \infty$. Therefore (ii) holds.

Now assume $f_\star = 0$, and let $\varepsilon > 0$ be arbitrary. By applying (i)⇒(ii) to the nc polynomial $f + \frac{n\varepsilon}{2}$ and $\frac{\varepsilon}{2} > 0$, there exists $r \in \mathbb{N}$ such that $\left(f + \frac{n\varepsilon}{2}\right) + \frac{\varepsilon}{2}\Omega_r \in \Theta^2_{2r}$. But this nc polynomial equals $f + \varepsilon\Omega_r - \frac{\varepsilon}{2}(\Omega_r - n)$, so $f + \varepsilon\Omega_r \in \Theta^2_{2r}$. □

Remark 7.7 Let $f \in \mathbb{R}\langle\underline{x}\rangle_{\rm sa}$. For $r \in \mathbb{N}$ let

$$\varepsilon_r = \inf\left\{\varepsilon \in \mathbb{R}\colon\ f + \varepsilon\Omega_r \in \Theta^2_{2r}\right\}.$$

Then $(\varepsilon_r)_r$ is a decreasing sequence, each ε_r can be computed with a semidefinite program, and f is trace-positive if and only if $\inf_r \varepsilon_r \leq 0$ by Theorem 7.2.

7.3 Sum-of-squares perturbations of the tracial Motzkin polynomial

We illustrate Theorem 7.2 on the polynomial $m = x_2x_1^4x_2 + x_2^2x_1^2x_2^2 - 3x_2x_1^2x_2 + 1 \in \mathbb{R}\langle x_1, x_2\rangle_{\mathrm{sa}}$ from Example 3.2. In fact, we show in Example 7.9 below that for every $\varepsilon > 0$ there is $r \in \mathbb{N}$ such that $m + \frac{\varepsilon}{r!}x_1^{2r}$ is cyclically equivalent to a sum of hermitian squares. This in particular improves the approximation of the commutative Motzkin polynomial by sums of squares given in [32, Example 3.5]. We start with a technical lemma.

Lemma 7.8 *Let $r \in 4\mathbb{N}+1$ and $\varepsilon \geq \frac{r!}{(r-1)^{r-1}}$. Then the polynomial*

$$p(t) = -\left(\frac{t-r}{r-1}\right)^{\frac{r-1}{2}}$$

satisfies

$$2p(t) \leq t-3 \quad \text{and} \quad tp(t)^2 \leq 1 + \frac{\varepsilon}{r!}t^r$$

for all $t \geq 0$.

Proof Observe that p is concave on $\mathbb{R}$ (since $\frac{r-1}{2}$ is even), $p(1) = -1$ and $p'(1) = \frac{1}{2}$. Therefore $p(t) \leq \frac{1}{2}(t-3)$ for all $t \in \mathbb{R}$.

On $(0,\infty)$, the function $t \mapsto t(t-1)^{r-1}$ has precisely two local extrema, a local maximum at $\frac{1}{r}$ and a local minimum at 1. Therefore

$$t(t-1)^{r-1} - \frac{1}{r}\left(\frac{1}{r}-1\right)^{r-1} \leq t^r$$

for all $t \geq 0$. Replacing t with $\frac{t}{r}$ gives

$$\left(\frac{t}{r}\right)\left(\left(\frac{t}{r}\right)-1\right)^{r-1} \leq \frac{1}{r}\left(\frac{1}{r}-1\right)^{r-1} + \left(\frac{t}{r}\right)^r,$$

and after multiplication by $\frac{r^r}{(r-1)^{r-1}}$ we obtain

$$t\left(\frac{t-r}{r-1}\right)^{r-1} \leq 1 + \frac{t^r}{(r-1)^{r-1}}.$$

Therefore $tp(t)^2 \leq 1 + \frac{\varepsilon}{r!}t^r$ holds for all $t \geq 0$. □

Example 7.9 Let $M = t_1^4 t_2^2 + t_1^2 t_2^4 - 3t_1^2 t_2^2 + 1 \in \mathbb{R}[t_1, t_2]$ be the Motzkin polynomial. If $r \in 4\mathbb{N}+1$ and $\varepsilon \geq \frac{r!}{(r-1)^{r-1}}$, then $M + \frac{\varepsilon}{r!} t_1^{2r}$ is a sum of squares in $\mathbb{R}[t_1, t_2]$. Note that $\frac{r!}{(r-1)^{r-1}}$ decays exponentially towards 0 as $r \to \infty$.

Indeed, let p be as in Lemma 7.8. The univariate polynomials $t_1^4 - 3t_1^2 - 2t_1^2 p(t_1^2)$ and $1 + \frac{\varepsilon}{r!} t_1^{2r} - t_1^2 p(t_1^2)^2$ are nonnegative, and therefore sums of squares in $\mathbb{R}[t_1]$. Then

$$\begin{aligned} M + \frac{\varepsilon}{r!} t_1^{2r} &= t_1^2 t_2^4 + (t_1^4 - 3t_1^2) t_2^2 + \left(1 + \frac{\varepsilon}{r!} t_1^{2r}\right) \\ &= \left(t_1^4 - 3t_1^2 - 2t_1^2 p(t_1^2)\right) t_2^2 + t_1^2 \left(t_2^2 + p(t_1^2)\right)^2 + \left(1 + \frac{\varepsilon}{r!} t_1^{2r} - t_1^2 p(t_1^2)^2\right) \end{aligned}$$

is a sum of (at most five) squares in $\mathbb{R}[t_1, t_2]$.

Let $m \in \mathbb{R}\langle x_1, x_2 \rangle_{\mathrm{sa}}$ be a cyclically sorted noncommutative lift of M. As in the proof of Corollary 5.4 we conclude that

$$m + \frac{\varepsilon}{r!} x_1^{2r} \in \Theta_{2r}^2$$

for $r \in 4\mathbb{N}+1$ and $\varepsilon \geq \frac{r!}{(r-1)^{r-1}}$. □

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References

1. Alekseev, V., Netzer, T., Thom, A.: Quadratic modules, C^*-algebras, and free convexity. Trans. Am. Math. Soc. **372**, 7525–7539 (2019)
2. Barvinok, A.: A Course in Convexity, Graduate Studies in Mathematics 54. American Mathematical Society, Providence (2002)
3. Beigi, S.: Sandwiched Rényi divergence satisfies data processing inequality. J. Math. Phys. **54**, 122202 (2013)
4. Beutner, E.: On the closedness of the sum of closed convex cones in reflexive Banach spaces. J. Convex Anal. **14**, 99–102 (2007)
5. Bhatia, R.: Matrix Analysis, Graduate Texts in Mathematics 169. Springer, New York (1997)
6. Burgdorf, S., Klep, I., Povh, J.: Optimization of Polynomials in Non-commuting Variables. Springer Briefs in Mathematics. Springer, Cham (2016)
7. Carlen, E.: Trace Inequalities and Quantum Entropy: An Introductory Course, Entropy and the Quantum, Contemp. Math. 529, pp. 73–140. American Mathematical Society, Providence (2010)
8. Cimprič, J., Marshall, M., Netzer, T.: Closures of quadratic modules. Israel J. Math. **183**, 445–474 (2011)
9. Cohn, P.M.: Skew Fields. Theory of General Division Rings, Encyclopedia of Mathematics and Its Applications 57. Cambridge University Press, Cambridge (1995)
10. Collins, B., Dykema, K.J.: A linearization of Connes' embedding problem. N. Y. J. Math. **14**, 617–641 (2008)
11. Curto, R.E., Fialkow, L.A.: Flat extensions of positive moment matrices: recursively generated relations. Mem. Am. Math. Soc. **136**, 648 (1998)
12. Dubois-Violette, M.: A generalization of the classical moment problem on $*$-algebras with applications to relativistic quantum theory I. Commun. Math. Phys. **43**, 225–254 (1975)

13. Dykema, K.J.: Factoriality and Connes' invariant $T(\mathcal{M})$ for free products of von Neumann algebras. J. Reine Angew. Math. **450**, 159–180 (1994)
14. Fack, T., Kosaki, H.: Generalized s-numbers of τ-measurable operators. Pacific J. Math. **123**, 269–300 (1986)
15. Fritz, T., Netzer, T., Thom, A.: Can you compute the operator norm? Proc. Am. Math. Soc. **142**, 4265–4276 (2014)
16. Gribling, S., de Laat, D., Laurent, M.: Lower bounds on matrix factorization ranks via noncommutative polynomial optimization. Found. Comput. Math. **19**, 1013–1070 (2019)
17. Grinshpan, A., Kaliuzhnyi-Verbovetskyi, D.S., Vinnikov, V., Woerdeman, H.J.: Matrix-valued Hermitian Positivstellensatz, lurking contractions, and contractive determinantal representations of stable polynomials, Operator theory, function spaces, and applications. Oper. Theory Adv. Appl. **255**, 123–136 (2016). (**Birkhäuser/Springer, Cham**)
18. Guionnet, A., Shlyakhtenko, D.: Free diffusions and matrix models with strictly convex interaction. Geom. Funct. Anal. **18**, 1875–1916 (2009)
19. Hadwin, D.: A noncommutative moment problem. Proc. Am. Math. Soc. **129**, 1785–1791 (2001)
20. Helton, J.W.: Positive noncommutative polynomials are sums of squares. Ann. Math. **156**, 675–694 (2002)
21. Helton, J.W., McCullough, S.: A Positivstellensatz for non-commutative polynomials. Trans. Am. Math. Soc. **356**, 3721–3737 (2004)
22. Inoue, A.: On a class of unbounded operator algebras II. Pacific J. Math. **66**, 411–431 (1976)
23. Z. Ji, A. Natarajan, T. Vidick, J. Wright, H. Yuen: MIP* = RE. Commun. ACM 64, 131–138 (2021). arXiv:2001.04383
24. Junge, M., Zeng, Q.: Noncommutative Bennett and Rosenthal inequalities. Ann. Probab. **41**, 4287–4316 (2013)
25. Klep, I., Magron, V., Volčič, J.: Optimization over trace polynomials. Ann. Henri Poincaré **23**, 67–100 (2022)
26. Klep, I., Pascoe, J.E., Volčič, J.: Regular and positive noncommutative rational functions. J. Lond. Math. Soc. (2) **95**, 613–632 (2017)
27. Klep, I., Pascoe, J.E., Volčič, J.: Positive univariate trace polynomials. J. Algebra **579**, 303–317 (2021)
28. Klep, I., Schweighofer, M.: Connes' embedding conjecture and sums of hermitian squares. Adv. Math. **217**, 1816–1837 (2008)
29. Klep, I., Špenko, Š, Volčič, J.: Positive trace polynomials and the universal Procesi-Schacher conjecture. Proc. Lond. Math. Soc. (3) **117**, 1101–1134 (2018)
30. Kosaki, H.: An inequality of Araki-Lieb-Thirring (von Neumann algebra case). Proc. Am. Math. Soc. **114**, 477–481 (1992)
31. Lasserre, J.B.: A sum of squares approximation of nonnegative polynomials. SIAM J. Optim. **16**, 751–765 (2006)
32. Lasserre, J.B., Netzer, T.: SOS approximations of nonnegative polynomials via simple high degree perturbations. Math. Z. **256**, 99–112 (2007)
33. Laurent, M.: Sums of Squares, Moment Matrices and Optimization, in Emerging Applications of Algebraic Geometry, 157–270, IMA Volumes in Mathematics and its Applications 149. Springer, Berlin (2009)
34. Lieb, E.H., Thirring, W.E.: ,Inequalities for the Moments of the Eigenvalues of the Schrödinger Hamiltonian and Their Relation to Sobolev Inequalities, in Studies in Mathematical Physics, pp. 269–303. Princeton University Press, Princeton (1976)
35. Marshall, M.: Positive Polynomials and Sums of Squares, Mathematical Surveys and Monographs 146. American Mathematical Society, Providence (2008)
36. McCullough, S.: Factorization of operator-valued polynomials in several non-commuting variables. Linear Algebra Appl. **326**, 193–203 (2001)
37. Mingo, J.A., Speicher, R.: Free Probability and Random Matrices, Fields Institute Monographs 35. Springer, New York (2017)
38. Nelson, E.: Notes on non-commutative integration. J. Funct. Anal. **15**, 103–116 (1974)
39. Netzer, T., Thom, A.: Tracial algebras and an embedding theorem. J. Funct. Anal. **259**, 2939–2960 (2010)
40. Ozawa, N.: About the Connes embedding conjecture: algebraic approaches. Jpn. J. Math. **8**, 147–183 (2013)

41. Pozas-Kerstjens, A., Rabelo, R., Rudnicki, L., Chaves, R., Cavalcanti, D., Navascués, M., Acín, A.: Bounding the sets of classical and quantum correlations in networks. Phys. Rev. Lett. **123**, 140503 (2019)
42. Procesi, C., Schacher, M.: A non-commutative real Nullstellensatz and Hilbert's 17th problem. Ann. Math. **104**, 395–406 (1976)
43. Putinar, M., Vasilescu, F.-H.: Solving moment problems by dimensional extension. Ann. Math. (2) **149**, 1087–1107 (1999)
44. Quarez, R.: Trace-positive non-commutative polynomials. Proc. Am. Math. Soc. **143**, 3357–3370 (2015)
45. Rădulescu, F.: A non-commutative, analytic version of Hilbert's 17th problem in type II_1 von Neumann algebras, Von Neumann algebras in Sibiu. Theta Ser. Adv. Math. **10**, 93–101 (2008). (**Theta, Bucharest**)
46. Reznick, B.: Uniform denominators in Hilbert's seventeenth problem. Math. Z. **220**, 75–97 (1995)
47. Reznick, B.: On the absence of uniform denominators in Hilbert's 17th problem. Proc. Am. Math. Soc. **133**, 2829–2834 (2005)
48. Scheiderer, C.: Sums of squares on real algebraic surfaces. Manuscripta Math. **119**, 395–410 (2006)
49. Scheiderer, C.: Positivity and Sums of Squares: A Guide to Recent Results, in Emerging Applications of Algebraic Geometry, IMA Volumes in Mathematics and its Applications 149, pp. 271–324. Springer, Berlin (2009)
50. Scheiderer, C.: A Positivstellensatz for projective real varieties. Manuscripta Math. **138**, 73–88 (2012)
51. Scheiderer, C., Wenzel, S.: Polynomials nonnegative on the cylinder. Contemp. Math. **697**, 291–300 (2017)
52. Schmüdgen, K.: Unbounded Self-adjoint Operators on Hilbert Space. Springer, New York (2012)
53. Schmüdgen, K.: The Moment Problem. Springer International Publishing AG, New York (2017)
54. Sutter, D., Berta, M., Tomamichel, M.: Multivariate trace inequalities. Commun. Math. Phys. **352**, 37–58 (2017)
55. Takesaki, M.: Theory of Operator Algebras II, Encyclopaedia of Mathematical Sciences 125. Springer, New York (2003)
56. Voiculescu, D.V.: The analogues of entropy and of Fisher's information measure in free probability theory, II. Invent. Math. **118**, 411–440 (1994)
57. Voiculescu, D.V., Dykema, K.J., Nica, A.: Free Random Variables. A Noncommutative Probability Approach to Free Products with Applications to Random Matrices, Operator Algebras and Harmonic Analysis on Free Groups, CRM Monograph Series 1. American Mathematical Society, Providence (1992)
58. Volčič, J.: Matrix coefficient realization theory of noncommutative rational functions. J. Algebra **499**, 397–437 (2018)