

CONSTRAINED POLYNOMIAL OPTIMIZATION PROBLEMS WITH NONCOMMUTING VARIABLES

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ABSTRACT. In this paper we study *constrained* eigenvalue optimization of noncommutative (nc) polynomials, focusing on the polydisc and the ball. Our three main results are as follows: (1) an nc polynomial is nonnegative if and only if it admits a weighted sum of hermitian squares decomposition; (2) (eigenvalue) optima for nc polynomials can be computed using a *single* semidefinite program (SDP) – this sharply contrasts the commutative case where *sequences* of SDPs are needed; (3) the dual solution to this “single” SDP can be exploited to extract eigenvalue optimizers with an algorithm based on two ingredients:

- solution to a *truncated nc moment problem* via flat extensions;
- Gelfand-Naimark-Segal (*GNS*) *construction*.

The implementation of these procedures in our computer algebra system `NCSOStools` is presented and several examples pertaining to matrix inequalities are given to illustrate our results.

1. INTRODUCTION

Starting with Helton’s seminal paper [Hel02], *free real algebraic geometry* is being established. Unlike classical real algebraic geometry where real polynomial rings in *commuting* variables are the objects of study, free real algebraic geometry deals with real polynomials in *noncommuting* (nc) variables and their finite-dimensional representations. Of interest are notions of *positivity* induced by these. For instance, positivity via positive semidefiniteness, which can be reformulated and studied using sums of hermitian squares and semidefinite programming. In the sequel we will use SDP to abbreviate semidefinite programming as the subarea of nonlinear optimization as well as to refer to an instance of semidefinite programming problems.

1.1. Motivation. Among the things that make this area exciting are its many facets of applications. Let us mention just a few. A nice survey on applications to control theory, systems engineering and optimization is given by Helton, McCullough, Oliveira, Putinar [HMdOP08], applications to quantum physics are explained by Pironio, Navascués, Acín [PNA10] who also consider computational aspects related so noncommutative sum of squares. For instance, optimization of nc polynomials has direct applications in quantum information science (to compute upper bounds on the maximal violation of a generic Bell inequality [PV09]), and also in quantum chemistry (e.g. to compute the ground-state electronic energy of atoms or molecules, cf. [Maz04]). Certificates of positivity via sums of squares are often used in the theoretical physics literature to place very general bounds on quantum correlations (cf. [Gla63]). Furthermore, the important Bessis-Moussa-Villani conjecture (BMV) from quantum statistical

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mechanics is tackled in [KS08b] and by the authors in [CKP10]. How this pertains to operator algebras is discussed by Schweighofer and the second author in [KS08a], Doherty, Liang, Toner, Wehner [DLTW08] employ free real algebraic geometry (or *free positivity*) to consider the quantum moment problem and multi-prover games.

We developed `NCSOSTools` [CKP11] as a consequence of this recent interest in free positivity and sums of (hermitian) squares (*sohs*). `NCSOSTools` is an open source Matlab toolbox for solving sohs problems using *semidefinite programming* (SDP). As a side product our toolbox implements symbolic computation with noncommuting variables in Matlab. Hence there is a small overlap in features with Helton’s `NCAAlgebra` package for Mathematica [HMdOS]. However, `NCSOSTools` performs only basic manipulations with noncommuting variables, while `NCAAlgebra` is a fully-fledged add-on for symbolic computation with polynomials, matrices and rational functions in noncommuting variables.

Readers interested in solving sums of squares problems for commuting polynomials are referred to one of the many great existing packages, such as GloptiPoly [HLL09], SOSTOOLS [PPSP05], SparsePOP [WKK⁺09], or YALMIP [Löf04].

1.2. Contribution. This article adds on to the list of properties that are much cleaner in the noncommutative setting than their commutative counterparts. For example: a positive semidefinite nc polynomial is a sum of squares [Hel02], a convex nc semialgebraic set has an LMI representation [HM], proper nc maps are one-to-one [HKM11], etc. More precisely, the purpose of this article is threefold.

First, we shall show that every noncommutative (nc) polynomial that is merely positive semidefinite on a ball or a polydisc admits a sum of hermitian squares representation with weights and tight degree bounds (*Nichtnegativstellensatz* 3.4). Note that this contrasts sharply with the commutative case, where *strict* positivity is needed and nevertheless there do not exist degree bounds, cf. [Sch09].

Second, we show how the existence of sharp degree bounds can be used to compute (eigenvalue) optima for nc polynomials on a ball or a polydisc by solving a *single* semidefinite programming problem (SDP). Again, this is much cleaner than the corresponding situation in the commutative setting, where *sequences* of SDPs are needed, cf. Lasserre’s relaxations [Las01, Las09].

Third, the dual solution of the SDP constructed above, can be exploited to extract eigenvalue optimizers. The algorithm is based on 1-step *flat extensions* of noncommutative Hankel matrices and the Gelfand-Naimark-Segal (GNS) construction, and *always* works – again contrasting the classical commutative case.

1.3. Reader’s guide. The paper starts with a preliminary section fixing notation, introducing terminology and stating some well-known classical results on positive nc polynomials (§2). We then proceed in §3 to establish our Nichtnegativstellensatz. The last two sections present computational aspects, including the construction and properties of the SDP computing the minimum of an nc polynomial in §4, and the extraction of optimizers in §5. We have implemented our algorithms in our open source Matlab toolbox `NCSOSTools` freely available at <http://ncsostools.fis.unm.si/>. Throughout the paper examples are given to illustrate our results and the use of our computer algebra package.

2. NOTATION AND PRELIMINARIES

2.1. Words, free algebras and nc polynomials. Fix $n \in \mathbb{N}$ and let $\langle \underline{X} \rangle$ be the monoid freely generated by $\underline{X} := (X_1, \dots, X_n)$, i.e., $\langle \underline{X} \rangle$ consists of *words* in the n noncommuting letters X_1, \dots, X_n (including the empty word denoted by 1). We consider the free algebra $\mathbb{R}\langle \underline{X} \rangle$. The elements of $\mathbb{R}\langle \underline{X} \rangle$ are linear combinations of words in the n letters \underline{X} and are called *noncommutative (nc) polynomials*. An element of the form aw where $a \in \mathbb{R} \setminus \{0\}$ and $w \in \langle \underline{X} \rangle$ is called a *monomial* and a its *coefficient*. Words are monomials with coefficient 1. The length of the longest word in an nc polynomial $f \in \mathbb{R}\langle \underline{X} \rangle$ is the *degree* of f and is denoted by $\deg f$. The set of all words and nc polynomials with degree $\leq d$ will be denoted by $\langle \underline{X} \rangle_d$ and $\mathbb{R}\langle \underline{X} \rangle_d$, respectively. If we are dealing with only two variables, we shall use X, Y instead of X_1, X_2 .

By \mathbb{S}_k we denote the set of all symmetric $k \times k$ real matrices and by \mathbb{S}_k^+ we denote the set of all real positive semidefinite $k \times k$ real matrices. Moreover, $\mathbb{S} := \bigcup_{k \in \mathbb{N}} \mathbb{S}_k$ and $\mathbb{S}^+ := \bigcup_{k \in \mathbb{N}} \mathbb{S}_k^+$. If A is positive semidefinite we denote this by $A \succeq 0$.

2.1.1. Sums of hermitian squares. We equip $\mathbb{R}\langle \underline{X} \rangle$ with the *involution* $*$ that fixes $\mathbb{R} \cup \{\underline{X}\}$ pointwise and thus reverses words, e.g. $(X_1 X_2^2 X_3 - 2X_3^3)^* = X_3 X_2^2 X_1 - 2X_3^3$. Hence $\mathbb{R}\langle \underline{X} \rangle$ is the $*$ -algebra freely generated by n symmetric letters. Let $\text{Sym } \mathbb{R}\langle \underline{X} \rangle$ denote the set of all *symmetric polynomials*,

$$\text{Sym } \mathbb{R}\langle \underline{X} \rangle := \{f \in \mathbb{R}\langle \underline{X} \rangle \mid f = f^*\}.$$

An nc polynomial of the form g^*g is called a *hermitian square* and the set of all sums of hermitian squares will be denoted by Σ^2 . Clearly, $\Sigma^2 \subsetneq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$. The involution $*$ extends naturally to matrices (in particular, to vectors) over $\mathbb{R}\langle \underline{X} \rangle$. For instance, if $V = (v_i)$ is a (column) vector of nc polynomials $v_i \in \mathbb{R}\langle \underline{X} \rangle$, then V^* is the row vector with components v_i^* . We use V^t to denote the row vector with components v_i .

We can stack all words from $\langle \underline{X} \rangle_d$ using the graded lexicographic order into a column vector W_d . The size of this vector will be denoted by $\sigma(d)$, hence

$$\sigma(d) := |W_d| = \sum_{k=0}^d n^k = \frac{n^{d+1} - 1}{n - 1}. \quad (1)$$

Every $f \in \mathbb{R}\langle \underline{X} \rangle_{2d}$ can be written (possible nonuniquely) as $f = W_d^* G_f W_d$, where $G_f = G_f^*$ is called a *Gram matrix* for f .

Example 2.1. Consider $f = 2 + XYXY + YXYX \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle$. Let

$$W_2 = [1 \quad X \quad Y \quad X^2 \quad XY \quad YX \quad Y^2]^t.$$

Then there are many $G_f \in \mathbb{S}_7$ satisfying $f = W_2^* G_f W_2$; for instance

$$G_f(u, v) = \begin{cases} 1 & \text{if } u^*v = XYXY \vee u^*v = YXYX \vee u^*v = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Obviously $f \notin \Sigma^2$ but we have

$$f = g_1^* g_1 + g_2^* g_2 + g_3^* g_3 + g_4^* g_4 + X(1 - X^2 - Y^2)X + Y(1 - X^2 - Y^2)Y, \quad (2)$$

where

$$g_1 = \sqrt{\frac{3}{2}}, \quad g_2 = \frac{\sqrt{2}}{2}(X^2 - Y^2), \quad g_3 = \frac{\sqrt{2}}{2}(1 - X^2 - Y^2), \quad g_4 = (XY + YX).$$

Alternately,

$$f = (XY + YX)^*(XY + YX) + (1 - X^2) + Y(1 - X^2)Y + (1 - Y^2) + X(1 - Y^2)X. \quad (3)$$

2.2. Nc semialgebraic sets and quadratic modules.

2.2.1. Nc semialgebraic sets.

Definition 2.2. Fix a subset $S \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$. The (operator) *semialgebraic set* \mathcal{D}_S^∞ associated to S is the class of tuples $\underline{A} = (A_1, \dots, A_n)$ of bounded self-adjoint operators on a Hilbert space making $s(\underline{A})$ a positive semidefinite operator for every $s \in S$. In case we are considering only tuples of symmetric matrices $\underline{A} \in \mathbb{S}^n$ satisfying $s(\underline{A}) \succeq 0$, we write \mathcal{D}_S . When considering symmetric matrices of a fixed size $k \in \mathbb{N}$, we shall use $\mathcal{D}_S(k) := \mathcal{D}_S \cap \mathbb{S}_k^n$.

We will focus on the two most important examples of nc semialgebraic sets:

Example 2.3.

(a) Let $S = \{1 - \sum_{i=1}^n X_i^2\}$. Then

$$\mathbb{B} := \bigcup_{k \in \mathbb{N}} \left\{ \underline{A} = (A_1, \dots, A_n) \in \mathbb{S}_k^n \mid 1 - \sum_{i=1}^n A_i^2 \succeq 0 \right\} = \mathcal{D}_S \quad (4)$$

is the *nc ball*. Note \mathbb{B} is the set of all row contractions of self-adjoint operators on finite-dimensional Hilbert spaces.

(b) Let $S = \{1 - X_1^2, \dots, 1 - X_n^2\}$. Then

$$\mathbb{D} := \bigcup_{k \in \mathbb{N}} \left\{ \underline{A} = (A_1, \dots, A_n) \in \mathbb{S}_k^n \mid 1 - A_1^2 \succeq 0, \dots, 1 - A_n^2 \succeq 0 \right\} = \mathcal{D}_S \quad (5)$$

is the *nc polydisc*. It consists of all n -tuples of self-adjoint contractions on finite-dimensional Hilbert spaces.

In the rest of the paper we will

- (§3) establish which nc polynomials f are positive semidefinite on \mathbb{B} and \mathbb{D} ;
- (§4) construct a *single* SDP which yields the smallest eigenvalue f attains on \mathbb{B} and \mathbb{D} ;
- (§5) use the solution of the dual SDP to compute an eigenvalue minimizer for f on \mathbb{B} and \mathbb{D} .

2.2.2. *Archimedean quadratic modules.* The main existing result in the literature concerning nc polynomials (strictly) positive on \mathbb{B} and \mathbb{D} is due to Helton and McCullough [HM04]. For a precise statement we recall (archimedean) quadratic modules.

Definition 2.4. A subset $M \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$ is called a **quadratic module** if

$$1 \in M, \quad M + M \subseteq M \quad \text{and} \quad a^* M a \subseteq M \quad \text{for all } a \in \mathbb{R}\langle \underline{X} \rangle.$$

Given a subset $S \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$, the quadratic module M_S generated by S is the smallest subset of $\text{Sym } \mathbb{R}\langle \underline{X} \rangle$ containing all $a^* s a$ for $s \in S \cup \{1\}$, $a \in \mathbb{R}\langle \underline{X} \rangle$, and closed under addition:

$$M_S = \left\{ \sum_{i=1}^N a_i^* s_i a_i \mid N \in \mathbb{N}, s_i \in S \cup \{1\}, a_i \in \mathbb{R}\langle \underline{X} \rangle \right\}.$$

The following is an obvious but important observation:

Proposition 2.5. *Let $S \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$. If $f \in M_S$, then $f|_{\mathcal{D}_S^\infty} \succeq 0$.*

The converse of Proposition 2.5 is false in general, i.e., nonnegativity on an nc semialgebraic set does not imply the existence of a weighted sum of squares certificate, cf. [KS07, Example 3.1]. A weak converse holds for *positive* nc polynomials under a strong *boundedness* assumption, see Theorem 2.7 below.

Definition 2.6. A quadratic module M is **archimedean** if

$$\forall a \in \mathbb{R}\langle \underline{X} \rangle \exists N \in \mathbb{N} : N - a^*a \in M. \quad (6)$$

Note if a quadratic module M_S is archimedean, then \mathcal{D}_S^∞ is bounded, i.e., there is an $N \in \mathbb{N}$ such that for every $\underline{A} \in \mathcal{D}_S^\infty$ we have $\|\underline{A}\| \leq N$. Examples of archimedean quadratic modules are obtained by generating them from defining sets for the nc ball and the nc polydisc.

2.2.3. A Positivstellensatz. The main result in the literature concerning archimedean quadratic modules is a theorem of Helton and McCullough. It is a perfect generalization of Putinar's Positivstellensatz [Put93] for commutative polynomials.

Theorem 2.7 (Helton & McCullough [HM04, Theorem 1.2]). *Let $S \cup \{f\} \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$ and suppose that M_S is archimedean. If $f(A) \succ 0$ for all $A \in \mathcal{D}_S^\infty$, then $f \in M_S$.*

We remark that if \mathcal{D}_S is nc convex [HM04, §2], then it suffices to check the positivity of f in Theorem 2.7 on \mathcal{D}_S , see [HM04, Proposition 2.3]. Our Nichtnegativstellensatz 3.4 will show that for \mathbb{B} and \mathbb{D} positive *semidefiniteness* of f is enough to establish the conclusion of Theorem 2.7. Under the absence of archimedeanity the conclusions of Theorem 2.7 may fail, cf. [KS07].

3. A NICHTNEGATIVSTELLENSATZ

The main result in this section is the Nichtnegativstellensatz 3.4. For a precise formulation we introduce truncated quadratic modules.

3.1. Truncated quadratic modules. Given a subset $S \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$, we introduce

$$\begin{aligned} \Sigma_S^2 &:= \left\{ \sum_i h_i^* s_i h_i \mid h_i \in \mathbb{R}\langle \underline{X} \rangle, s_i \in S \right\}, \\ \Sigma_{S,d}^2 &:= \left\{ \sum_i h_i^* s_i h_i \mid h_i \in \mathbb{R}\langle \underline{X} \rangle, s_i \in S, \deg(h_i^* s_i h_i) \leq 2d \right\}, \\ M_{S,d} &:= \left\{ \sum_i h_i^* s_i h_i \mid h_i \in \mathbb{R}\langle \underline{X} \rangle, s_i \in S \cup \{1\}, \deg(h_i^* s_i h_i) \leq 2d \right\}, \end{aligned} \quad (7)$$

and call $M_{S,d}$ the *truncated quadratic module* generated by S . Note $M_{S,d} = \Sigma_d^2 + \Sigma_{S,d}^2 \subseteq \mathbb{R}\langle \underline{X} \rangle_{2d}$, where $\Sigma_d^2 := M_{\emptyset,d}$ denotes the set of all sums of hermitian squares of polynomials of degree at most d . Furthermore, $M_{S,d}$ is a convex cone in the \mathbb{R} -vector space $\text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$. For example, if $S = \{1 - \sum_j X_j^2\}$ then $M_{S,d}$ contains exactly the polynomials f which have a *sum of hermitian squares (sohs) decomposition over the ball*, i.e., can be written as

$$f = \sum_i g_i^* g_i + \sum_i h_i^* \left(1 - \sum_{j=1}^n X_j^2\right) h_i, \quad \text{where} \quad (8)$$

$$\deg(g_i) \leq d, \quad \deg(h_i) \leq d - 1 \text{ for all } i.$$

Similarly, for $S = \{1 - X_1^2, 1 - X_2^2, \dots, 1 - X_n^2\}$, $M_{S,d}$ contains exactly the polynomials f which have a *sohs decomposition over the polydisc*, i.e., can be written as

$$f = \sum_i g_i^* g_i + \sum_{j=1}^n \sum_i h_{i,j}^* (1 - X_j^2) h_{i,j}, \quad \text{where} \quad (9)$$

$$\deg(g_i) \leq d, \quad \deg(h_{i,j}) \leq d - 1 \text{ for all } i, j.$$

We also call a decomposition of the form (8) or (9) a *sohs decomposition with weights*.

Example 3.1. Note the the polynomial f from Example 2.1 has a sohs decomposition over the ball, as follows from (2). Moreover, (3) implies that f also has a sohs decomposition over the polydisc.

Let us consider another example.

Example 3.2. Let $f = 2 - X^2 + XY^2X - Y^2 \in \text{Sym } \mathbb{R}\langle X \rangle$. Obviously $f \notin \Sigma^2$ but

$$f = (YX)^* YX + (1 - X^2) + (1 - Y^2), \quad (10)$$

i.e., f has a sohs decomposition over the polydisc, as well over the ball, since

$$f = 1 + (YX)^* YX + (1 - X^2 - Y^2). \quad (11)$$

Notation 3.3. For notational convenience, the truncated quadratic modules generated by the generator for the nc ball \mathbb{B} will be denoted by $M_{\mathbb{B},d}$, i.e.,

$$M_{\mathbb{B},d} := \left\{ \sum_i h_i^* s_i h_i \mid h_i \in \mathbb{R}\langle X \rangle, s_i \in \{1 - \sum_j X_j^2, 1\}, \deg(h_i^* s_i h_i) \leq 2d \right\} \subseteq \text{Sym } \mathbb{R}\langle X \rangle_{2d}, \quad (12)$$

Likewise, with $s_0 := 1$ and $s_i := 1 - X_i^2$,

$$M_{\mathbb{D},d} := \left\{ \sum_j \sum_{i=0}^n h_{i,j}^* s_i h_{i,j} \mid h_i \in \mathbb{R}\langle X \rangle, \deg(h_i^* s_i h_i) \leq 2d \right\} \subseteq \text{Sym } \mathbb{R}\langle X \rangle_{2d}. \quad (13)$$

3.2. Main result. Here is our main result. The rest of the section is devoted to its proof.

Theorem 3.4 (Nichtnegativstellensatz). *Let $f \in \mathbb{R}\langle X \rangle_{2d}$.*

- (1) $f|_{\mathbb{B}} \succeq 0$ if and only if $f \in M_{\mathbb{B},d+1}$.
- (2) $f|_{\mathbb{D}} \succeq 0$ if and only if $f \in M_{\mathbb{D},d+1}$.

By [HM04, §2], $f|_{\mathbb{B}} \succeq 0$ if and only if $f|_{\mathbb{B}(\sigma(d))} \succeq 0$. A similar statement holds for positive semidefiniteness on \mathbb{D} . These results will be reproved in the course of proving Theorem 3.4.

3.3. Proof of Theorem 3.4. To facilitate considering the two cases (the ball \mathbb{B} and the polydisc \mathbb{D}) simultaneously, we note they both contain an ε -neighborhood \mathcal{N}_ε of 0 for a small $\varepsilon > 0$. Here

$$\mathcal{N}_\varepsilon := \bigcup_{k \in \mathbb{N}} \left\{ \underline{A} = (A_1, \dots, A_n) \in \mathbb{S}_k^n \mid \varepsilon^2 - \sum_{i=1}^n A_i^2 \succeq 0 \right\}. \quad (14)$$

3.3.1. *A glance at polynomial identities.* The following lemma is a standard result in polynomial identities, cf. [Row80]. It is well known that there are no nonzero polynomial identities that hold for all sizes of (symmetric) matrices. In fact, it is enough to test on an ε -neighborhood of 0. An nc polynomial of degree $< 2d$ that vanishes on all n -tuples of symmetric matrices $\underline{A} \in \mathcal{N}_\varepsilon(N)^n$, for some $N \geq d$, is zero (this uses the standard multilinearization trick together with e.g. [Row80, §2.5, §1.4]).

Lemma 3.5. *If $f \in \mathbb{R}\langle \underline{X} \rangle$ is zero on \mathcal{N}_ε for some $\varepsilon > 0$, then $f = 0$.*

A variant of this lemma which we shall employ is as follows:

Proposition 3.6.

(1) *Suppose $f = \sum_i g_i^* g_i + \sum_i h_i^* (1 - \sum_j X_j^2) h_i \in M_{\mathbb{B},d}$. Then*

$$f|_{\mathbb{B}} = 0 \quad \Leftrightarrow \quad g_i = h_i = 0 \text{ for all } i.$$

(2) *Suppose $f = \sum_i g_i^* g_i + \sum_{i,j} h_{i,j}^* (1 - X_j^2) h_{i,j} \in M_{\mathbb{D},d}$. Then*

$$f|_{\mathbb{D}} = 0 \quad \Leftrightarrow \quad g_i = h_{i,j} = 0 \text{ for all } i, j.$$

Proof. We only need to prove the (\Rightarrow) implication, since (\Leftarrow) is obvious. We give the proof of (1); the proof of (2) is a verbatim copy.

Consider $f = \sum_i g_i^* g_i + \sum_i h_i^* (1 - \sum_j X_j^2) h_i \in M_{\mathbb{B},d}$ satisfying $f(\underline{A}) = 0$ for all $\underline{A} \in \mathbb{B}$. Let us choose $N > d$ and $\underline{A} \in \mathbb{B}(N)$. Obviously we have

$$g_i(\underline{A})^t g_i(\underline{A}) \succeq 0 \quad \text{and} \quad h_i(\underline{A})^t (1 - \sum_j A_j^2) h_i(\underline{A}) \succeq 0.$$

Since $f(\underline{A}) = 0$ this yields

$$g_i(\underline{A}) = 0 \quad \text{and} \quad h_i(\underline{A})^t (1 - \sum_j A_j^2) h_i(\underline{A}) = 0 \text{ for all } i.$$

By Lemma 3.5, $g_i = 0$ for all i . Likewise, $h_i^* (1 - \sum_j X_j^2) h_i = 0$ for all i . As there are no zero divisors in the free algebra $\mathbb{R}\langle \underline{X} \rangle$, the latter implies $h_i = 0$. \blacksquare

3.3.2. *Hankel matrices.*

Definition 3.7. To each linear functional $L : \mathbb{R}\langle \underline{X} \rangle_{2d} \rightarrow \mathbb{R}$ we associate a matrix H_L (called an *nc Hankel matrix*) indexed by words $u, v \in \langle \underline{X} \rangle_d$, with

$$(H_L)_{u,v} = L(u^* v). \tag{15}$$

If L is *positive*, i.e., $L(p^* p) \geq 0$ for all $p \in \mathbb{R}\langle \underline{X} \rangle_d$, then $H_L \succeq 0$.

Given $g \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle$, we associate to L the *localizing matrix* $H_{L,g}^{\text{shift}}$ indexed by words $u, v \in \langle \underline{X} \rangle_{d-\deg(g)/2}$ with

$$(H_{L,g}^{\text{shift}})_{u,v} = L(u^* g v). \tag{16}$$

If $L(h^* g h) \geq 0$ for all h with $h^* g h \in \mathbb{R}\langle \underline{X} \rangle_{2d}$ then $H_{L,g}^{\text{shift}} \succeq 0$.

We say that L is *unital* if $L(1) = 1$.

Remark 3.8. Note that a matrix H indexed by words of length $\leq d$ satisfying the *nc Hankel condition* $H_{u_1, v_1} = H_{u_2, v_2}$ whenever $u_1^* v_1 = u_2^* v_2$, gives rise to a linear functional L on $\mathbb{R}\langle \underline{X} \rangle_{2d}$ as in (15). If $H \succeq 0$, then L is positive.

Definition 3.9. Let $A \in \mathbb{R}^{s \times s}$ be a symmetric matrix. A (symmetric) extension of A is a symmetric matrix $\tilde{A} \in \mathbb{R}^{(s+\ell) \times (s+\ell)}$ of the form

$$\tilde{A} = \begin{bmatrix} A & B \\ B^t & C \end{bmatrix}$$

for some $B \in \mathbb{R}^{s \times \ell}$ and $C \in \mathbb{R}^{\ell \times \ell}$. Such an extension is *flat* if $\text{rank } A = \text{rank } \tilde{A}$, or, equivalently, if $B = AZ$ and $C = Z^tAZ$ for some matrix Z .

For later reference we record the following easy linear algebra fact.

Lemma 3.10. $\begin{bmatrix} A & B \\ B^t & C \end{bmatrix} \succeq 0$ if and only if $A \succeq 0$, and there is some Z with $B = AZ$ and $C \succeq Z^tAZ$.

3.3.3. GNS construction. Suppose $L : \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$ is a linear functional and let $\check{L} : \mathbb{R}\langle \underline{X} \rangle_{2d} \rightarrow \mathbb{R}$ denote its restriction. As in Definition 3.7 we associate to L and \check{L} the Hankel matrices H_L and $H_{\check{L}}$, respectively. In block form,

$$H_L = \begin{bmatrix} H_{\check{L}} & B \\ B^t & C \end{bmatrix}. \quad (17)$$

If H_L is flat over $H_{\check{L}}$, we call L (1-step) *flat*.

Proposition 3.11. Suppose $L : \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$ is positive and flat. Then there is an n -tuple \underline{A} of symmetric matrices of size $s \leq \sigma(d) = \dim \mathbb{R}\langle \underline{X} \rangle_d$ and a vector $\xi \in \mathbb{R}^s$ such that

$$L(p^*q) = \langle p(\underline{A})\xi, q(\underline{A})\xi \rangle \quad (18)$$

for all $p, q \in \mathbb{R}\langle \underline{X} \rangle$ with $\deg p + \deg q \leq 2d$.

Proof. For this we use the Gelfand-Naimark-Segal (GNS) construction. Let $H_L, \check{L}, H_{\check{L}}$ be as above. Note H_L (and hence $H_{\check{L}}$) is positive semidefinite. Since H_L is flat over $H_{\check{L}}$, there exist s linearly independent columns of $H_{\check{L}}$ labeled by words $w \in \langle \underline{X} \rangle$ with $\deg w \leq d$ which form a basis \mathcal{B} of $E = \text{Ran } H_L$. Now L (or, more precisely, H_L) induces a positive definite bilinear form (i.e., a scalar product) $\langle \cdot, \cdot \rangle_E$ on E .

Let A_i be the left multiplication with X_i on E , i.e., if \bar{w} denotes the column of H_L labeled by $w \in \langle \underline{X} \rangle_{d+1}$, then $A_i : \bar{u} \mapsto \bar{X}_i u$ for $u \in \langle \underline{X} \rangle_d$. The operator A_i is well defined and symmetric:

$$\langle A_i \bar{p}, \bar{q} \rangle_E = L(p^* X_i q) = \langle \bar{p}, A_i \bar{q} \rangle_E.$$

Let $\xi := \bar{1}$, and $\underline{A} = (A_1, \dots, A_n)$. Note it suffices to prove (18) for words $u, w \in \langle \underline{X} \rangle$ with $\deg u + \deg w \leq 2d$. Since the A_i are symmetric, there is no harm in assuming $\deg u, \deg w \leq d$. Now compute

$$L(u^*w) = \langle \bar{u}, \bar{w} \rangle_E = \langle u(\underline{A})\bar{1}, w(\underline{A})\bar{1} \rangle_E = \langle u(\underline{A})\xi, w(\underline{A})\xi \rangle_E. \quad \blacksquare$$

3.3.4. Separation argument. The following technical proposition is a variant of a Powers-Scheiderer result [PS01, §2].

Proposition 3.12. $M_{\mathbb{B},d}$ and $M_{\mathbb{D},d}$ are closed convex cones in the finite dimensional real vector space $\text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$.

Proof. We shall consider the case of the nc ball, whence let $S = \{1 - \sum_i X_i^2\}$; the proof for the polydisc is similar. By Carathéodory's theorem on convex hulls, each element of $M_{S,d}$ can be written as the sum of at most $m := \sigma(d) + 1$ terms of the form g^*g and $h^*(1 - \sum_{i=1}^n X_i^2)h$ where $g \in \mathbb{R}\langle \underline{X} \rangle_d$, $h \in \mathbb{R}\langle \underline{X} \rangle_{d-1}$. Hence $M_{S,d}$ is the image of the map

$$\Phi : \begin{cases} \mathbb{R}\langle \underline{X} \rangle_d^{m+1} \times \mathbb{R}\langle \underline{X} \rangle_{d-1}^{m+1} \rightarrow \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d} \\ (g_1, \dots, g_{m+1}, h_1, \dots, h_{m+1}) \mapsto \sum_{j=1}^{m+1} g_j^* g_j + \sum_{j=1}^{m+1} h_j^* (1 - \sum_{i=1}^n X_i^2) h_j. \end{cases}$$

We claim that $\Phi^{-1}(0) = \{0\}$. If $f = \sum_{j=1}^{m+1} g_j^* g_j + \sum_{j=1}^{m+1} h_j^* (1 - \sum_{i=1}^n X_i^2) h_j = 0$, then Proposition 3.6 shows $g_j = 0 = h_j$ for all j . This proves that $\Phi^{-1}(0) = \{0\}$. Together with the fact that Φ is homogeneous [PS01, Lemma 2.7], this implies that Φ is a proper and therefore a closed map. In particular, its image $M_{S,d}$ is closed in $\text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$. ■

3.3.5. Concluding the proof of Theorem 3.4. We now have all the tools needed to prove the Nichtnegativstellensatz 3.4. We prove (1) and leave (2) as an exercise for the reader. The implication (\Leftarrow) is trivial (cf. Proposition 2.5), so we only consider the converse.

Assume $f \notin M_{\mathbb{B},d+1}$. By the Hahn-Banach separation theorem and Proposition 3.12, there is a linear functional

$$L : \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R} \quad (19)$$

satisfying

$$L(M_{\mathbb{B},d+1}) \subseteq [0, \infty), \quad L(f) < 0. \quad (20)$$

Let $\check{L} := L|_{\mathbb{R}\langle \underline{X} \rangle_{2d}}$.

Lemma 3.13. *There is a positive flat linear functional $\hat{L} : \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$ extending \check{L} .*

Proof. Consider the Hankel matrix H_L presented in block form

$$H_L = \begin{bmatrix} H_{\check{L}} & B \\ B^t & C \end{bmatrix}.$$

The top left block $H_{\check{L}}$ is indexed by words of degree $\leq d$, and the bottom right block C is indexed by words of degree $d+1$.

We shall modify C to make the new matrix flat over $H_{\check{L}}$. By Lemma 3.10, there is some Z with $B = H_{\check{L}}Z$ and $C \succeq Z^t H_{\check{L}} Z$. Let us form

$$H = \begin{bmatrix} H_{\check{L}} & B \\ B^t & Z^t H_{\check{L}} Z \end{bmatrix}.$$

Then $H \succeq 0$ and H is flat over $H_{\check{L}}$ by construction. It also satisfies the Hankel constraints (cf. Remark 3.8), since there are no constraints in the bottom right block. (Note: this uses the noncommutativity and the fact that we are considering only extensions of one degree.) Thus H is a Hankel matrix of a positive linear functional $\hat{L} : \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$ which is flat. ■

The linear functional \hat{L} satisfies the assumptions of Proposition 3.11. Hence there is an n -tuple \underline{A} of symmetric matrices of size $s \leq \sigma(d)$ and a vector $\xi \in \mathbb{R}^s$ such that

$$\hat{L}(p^*q) = \langle p(\underline{A})\xi, q(\underline{A})\xi \rangle$$

for all $p, q \in \mathbb{R}\langle \underline{X} \rangle$ with $\deg p + \deg q \leq 2d$. By linearity,

$$\langle f(\underline{A})\xi, \xi \rangle = \hat{L}(f) = L(f) < 0. \quad (21)$$

It remains to be seen that \underline{A} is a row contraction, i.e., $1 - \sum_j A_j^2 \succeq 0$. For this we need to recall the construction of the A_j from the proof of Proposition 3.11.

Let $E = \text{Ran } H_{\hat{L}}$. There exist s linearly independent columns of $H_{\hat{L}}$ labeled by words $w \in \langle \underline{X} \rangle$ with $\deg w \leq d$ which form a basis \mathcal{B} of E . The scalar product on E is induced by \hat{L} , and A_i is the left multiplication with X_i on E , i.e., $A_i: \bar{u} \mapsto \overline{X_i u}$ for $u \in \langle \underline{X} \rangle_d$.

Let $\bar{u} \in E$ be arbitrary. Then there are $\alpha_v \in \mathbb{R}$ for $v \in \langle \underline{X} \rangle_d$ with

$$\bar{u} = \sum_{v \in \langle \underline{X} \rangle_d} \alpha_v \bar{v}.$$

Write $u = \sum_v \alpha_v v \in \mathbb{R} \langle \underline{X} \rangle_d$. Now compute

$$\begin{aligned} \langle (1 - \sum_j A_j^2) \bar{u}, \bar{u} \rangle &= \sum_{v, v' \in \langle \underline{X} \rangle_d} \alpha_v \alpha_{v'} \langle (1 - \sum_j A_j^2) \bar{v}, \bar{v}' \rangle \\ &= \sum_{v, v'} \alpha_v \alpha_{v'} \langle \bar{v}, \bar{v}' \rangle - \sum_{v, v'} \alpha_v \alpha_{v'} \sum_j \langle A_j \bar{v}, A_j \bar{v}' \rangle \\ &= \sum_{v, v'} \alpha_v \alpha_{v'} \hat{L}(v'^* v) - \sum_{v, v'} \alpha_v \alpha_{v'} \sum_j \hat{L}(v'^* X_j^2 v) \\ &= \hat{L}(u^* u) - \sum_j \hat{L}(u^* X_j^2 u) = L(u^* u) - \sum_j \hat{L}(u^* X_j^2 u). \end{aligned} \tag{22}$$

Here, the last equality follows from the fact that $\hat{L}|_{\mathbb{R} \langle \underline{X} \rangle_{2d}} = \check{L} = L|_{\mathbb{R} \langle \underline{X} \rangle_{2d}}$. We now estimate the summands $\hat{L}(u^* X_j^2 u)$:

$$\hat{L}(u^* X_j^2 u) = H_{\hat{L}}(X_j u, X_j u) \leq H_L(X_j u, X_j u) = L(u^* X_j^2 u). \tag{23}$$

Using (23) in (22) yields

$$\begin{aligned} \langle (1 - \sum_j A_j^2) \bar{u}, \bar{u} \rangle &= L(u^* u) - \sum_j \hat{L}(u^* X_j^2 u) \\ &\geq L(u^* u) - \sum_j L(u^* X_j^2 u) = L(u^* (1 - \sum_j X_j^2) u) \geq 0, \end{aligned}$$

where the last inequality is a consequence of (20).

All this shows that \underline{A} is a row contraction, that is, $\underline{A} \in \mathbb{B}$. As in (21),

$$\langle f(\underline{A}) \xi, \xi \rangle = L(f) < 0,$$

contradicting our assumption $f|_{\mathbb{B}} \succeq 0$ and finishing the proof of Theorem 3.4. \blacksquare

We note that a slightly different (and less self-contained) proof of Theorem 3.4 might be given by combining our Lemma 3.13 with [PNA10, Theorem 2].

4. OPTIMIZATION OF NC POLYNOMIALS IS A SINGLE SDP

In this section we thoroughly explain how eigenvalue optimization of an nc polynomial over the ball or polydisc is a *single* SDP.

4.1. Semidefinite Programming (SDP). Semidefinite programming (SDP) is a subfield of convex optimization concerned with the optimization of a linear objective function over the intersection of the cone of positive semidefinite matrices with an affine space [Nem07, BTN01, VB96]. The importance of semidefinite programming was spurred by the development of efficient (e.g. interior point) methods which can find an ε -optimal solution in a polynomial time in s, m and $\log \varepsilon$, where s is the order of the matrix variables m is the number of linear constraints. There exist several open source packages which find such solutions in practice. If

the problem is of medium size (i.e., $s \leq 1000$ and $m \leq 10.000$), these packages are based on interior point methods (see e.g. [dK02, NT08]), while packages for larger semidefinite programs use some variant of the first order methods (cf. [MPRW09, WGY10]). For a comprehensive list of state of the art SDP solvers see [Mit03].

4.1.1. *SDP and nc polynomials.* Let $S \subseteq \text{Sym } \mathbb{R}\langle \underline{X} \rangle$ be finite and let $f \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$. We are interested in the smallest eigenvalue $f_\star \in \mathbb{R}$ the polynomial f can attain on \mathcal{D}_S , i.e.,

$$f_\star := \inf \{ \langle f(\underline{A})\xi, \xi \rangle \mid \underline{A} \in \mathcal{D}_S, \xi \text{ a unit vector} \}. \quad (24)$$

Hence f_\star is the greatest lower bound on the eigenvalues of $f(\underline{A})$ for tuples of symmetric matrices $\underline{A} \in \mathcal{D}_S$, i.e., $(f - f_\star)(\underline{A}) \succeq 0$ for all $\underline{A} \in \mathcal{D}_S$, and f_\star is the largest real number with this property.

From Proposition 2.5 it follows that we can bound f_\star from below as follows

$$f_\star \geq \underset{\text{s. t.}}{f_{\text{sohs}}^{(s)}} := \sup \lambda \quad (\text{SPSDP}_{\text{eig-min}})$$

$$\text{s. t.} \quad f - \lambda \in M_{S,s},$$

for $s \geq d$. For each *fixed* s this is an SDP and leads to the noncommutative version of the Lasserre relaxation scheme, cf. [PNA10]. However, as a consequence of the Nichtnegativstellensatz 3.4, if \mathcal{D}_S is the ball \mathbb{B} or the polydisc \mathbb{D} then we do *not* need *sequences* of SDPs, a *single* SDP suffices: the first step in the noncommutative SDP hierarchy is already exact.

4.2. **Optimization of nc polynomials over the ball.** In this subsection we consider $S = \{1 - \sum_{i=1}^n X_i^2\}$ and the corresponding nc semialgebraic set $\mathbb{B} = \mathcal{D}_S$, the so-called nc ball.

From Theorem 3.4 it follows that we can rephrase f_\star , the greatest lower bound on the eigenvalues of $f \in \mathbb{R}\langle \underline{X} \rangle_{2d}$ over the ball \mathbb{B} , as follows:

$$f_\star = f_{\text{sohs}} = \sup \lambda \quad (\text{PSDP}_{\text{eig-min}})$$

$$\text{s. t.} \quad f - \lambda \in M_{S,d+1}.$$

Remark 4.1. We note that $f_\star > -\infty$ since positive semidefiniteness of a polynomial $f \in \mathbb{R}\langle \underline{X} \rangle_{2d}$ on \mathbb{B} only needs to be tested on the compact set $\mathbb{B}(N)$ for some $N \geq \sigma(d)$.

Verifying whether $f \in M_{\mathbb{B},d}$ is a semidefinite programming feasibility problem:

Proposition 4.2. *Let $f = \sum_{w \in \langle \underline{X} \rangle_{2d}} f_w w$. Then $f \in M_{\mathbb{B},d}$ if and only there exist positive semidefinite matrices H and G of order $\sigma(d)$ and $\sigma(d-1)$, respectively, such that for all $w \in \langle \underline{X} \rangle_{2d}$,*

$$f_w = \sum_{\substack{u,v \in \langle \underline{X} \rangle_d \\ u^*v=w}} H(u,v) + \sum_{\substack{u,v \in \langle \underline{X} \rangle_{d-1} \\ u^*v=w}} G(u,v) - \sum_{j=1}^n \sum_{\substack{u,v \in \langle \underline{X} \rangle_{d-1} \\ u^*X_j^2v=w}} G(u,v). \quad (25)$$

Proof. By definition $M_{S,d}$ contains only nc polynomials of the form

$$\sum_i h_i^* h_i + \sum_i g_i^* \left(1 - \sum_j X_j^2 \right) g_i, \quad \deg h_i \leq d, \deg g_i \leq d-1.$$

If $f \in M_{S,d}$ then we can obtain from h_i, g_i column vectors G_i and H_i of length $\sigma(d)$ and $\sigma(d-1)$, respectively, such that $h_i = H_i^t W_d$ and $g_i = G_i^t W_{d-1}$. Let us define $H := \sum_i H_i H_i^t$

and $G := \sum_i G_i G_i^t$. It follows that

$$\begin{aligned}
f &= \sum_i W_d^* H_i H_i^t W_d + \sum_i W_{d-1}^* G_i (1 - \sum_j X_j^2) G_i^t W_{d-1} \\
&= W_d^* \left(\sum_i H_i H_i^t \right) W_d + W_{d-1}^* \left(\sum_i G_i G_i^t - \sum_j X_j \left(\sum_i G_i G_i^t \right) X_j \right) W_{d-1} \\
&= \underbrace{W_d^* H W_d}_{=:S_1} + \underbrace{W_{d-1}^* G W_{d-1}}_{=:S_2} - \underbrace{W_d^* \sum_{i,j} G_i^j (G_i^j)^t W_d}_{=:S_3},
\end{aligned} \tag{26}$$

where the column vectors G_i^j are defined by

$$G_i^j(u) = \begin{cases} G_i(v), & \text{if } u = X_j v, \\ 0, & \text{otherwise.} \end{cases}$$

We have to show that (26) is exactly (25), i.e., G and H are feasible for (25). Let us consider $\tilde{G} := \sum_{i,j} G_i^j (G_i^j)^t$. Suppose $w = u^* v$ for some $u, v \in \langle X \rangle_d$. Equation (26) implies that f_w is the sum of all coefficients corresponding to w in sums S_1 , S_2 and S_3 . The coefficient corresponding to w in S_1 is $\sum_{\substack{u,v \in W_d \\ u^* v = w}} H(u, v)$. If in addition $w \in \langle X \rangle_{2d-2}$, then w appears also

in the summand S_2 with coefficient $\sum_{\substack{u,v \in W_{d-1} \\ u^* v = w}} G(u, v)$. In the third summand S_3 appear exactly

the words w which can be decomposed as $w = u^* v = u_1^* X_j^2 v_1$ for some $1 \leq j \leq n$ and some $u_1, v_1 \in \langle X \rangle_{d-1}$. Such w have coefficients

$$\begin{aligned}
-\sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle X \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \tilde{G}(X_j u_1, X_j v_1) &= -\sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle X \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \sum_i G_i^j(X_j u_1) G_i^j(X_j v_1) \\
-\sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle X \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \sum_i G_i(u_1) G_i(v_1) &= -\sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle X \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} G(u_1, v_1).
\end{aligned}$$

Therefore matrices H and G are feasible for (25).

To prove the converse we start with rank one decompositions: $H = \sum_i H_i H_i^t$ and $G = \sum_i G_i G_i^t$. If we define $h_i = H_i^t W_d$ and $g_i = G_i^t W_{d-1}$ then feasibility of H and G for (25) implies

$$\begin{aligned}
&\sum_i h_i^* h_i + \sum_i g_i^* \left(1 - \sum_j X_j^2 \right) g_i = \\
&\sum_i \sum_{u,v \in \langle X \rangle_d} H_i(u) H_i(v) u^* v + \sum_i \sum_{u,v \in \langle X \rangle_{d-1}} \left(G_i(u) G_i(v) u^* v - \sum_j G_i(u) G_i(v) u^* X_j^2 v \right) \\
&= \sum_{w \in \langle X \rangle_{2d}} \sum_{\substack{u,v \in \langle X \rangle_d \\ u^* v = w}} H(u, v) w + \sum_{w \in \langle X \rangle_{2d-2}} \sum_{\substack{u,v \in \langle X \rangle_{d-1} \\ u^* v = w}} G(u, v) w - \sum_{w \in \langle X \rangle_{2d}} \sum_j \sum_{\substack{u,v \in \langle X \rangle_{d-1} \\ u^* X_j^2 v = w}} G(u, v) w \\
&= \sum_{w \in \langle X \rangle_{2d}} f_w w = f,
\end{aligned}$$

concluding the proof. \blacksquare

Remark 4.3. The last part of the proof of Proposition 4.2 explains how to construct the sohs decomposition with weights (8) for $f \in M_{\mathbb{B},d}$. First we solve semidefinite feasibility problem in the variables $H \in \mathbb{S}_{\sigma(d)}^+$, $G \in \mathbb{S}_{\sigma(d-1)}^+$ subject to constraints (25). Then we compute by Cholesky or eigenvalue decomposition vectors $H_i \in \mathbb{R}^{\sigma(d)}$ and $G_i \in \mathbb{R}^{\sigma(d-1)}$ such that $H = \sum_i H_i H_i^t$ and $G = \sum_i G_i G_i^t$. Polynomials h_i and g_i from (8) are computed as $h_i = H_i^t W_d$ and $g_i = G_i^t W_{d-1}$.

By Proposition 4.2, the problem ($\text{PSDP}_{\text{eig-min}}$) is a SDP; it can be reformulated as

$$\begin{aligned}
 f_{\text{sohs}} &= \sup f_1 - \langle E_{1,1}, H \rangle - \langle E_{1,1}, G \rangle \\
 \text{s. t.} \quad f_w &= \sum_{\substack{u,v \in \langle \underline{X} \rangle_{d+1} \\ u^* v = w}} H(u,v) + \sum_{\substack{u,v \in \langle \underline{X} \rangle_d \\ u^* v = w}} G(u,v) - \sum_{j=1}^n \sum_{\substack{u,v \in \langle \underline{X} \rangle_d \\ u^* X_j^2 v = w}} G(u,v), \\
 &\text{for all } 1 \neq w \in \langle \underline{X} \rangle_{2d+2}, \\
 &H \in \mathbb{S}_{\sigma(d+1)}^+, G \in \mathbb{S}_{\sigma(d)}^+.
 \end{aligned} \tag{PSDP'_{\text{eig-min}}}$$

The dual semidefinite program to ($\text{PSDP}_{\text{eig-min}}$) and ($\text{PSDP}'_{\text{eig-min}}$) is:

$$\begin{aligned}
 L_{\text{sohs}} &= \inf L(f) \\
 \text{s. t.} \quad &L : \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R} \quad \text{is linear} \\
 &L(1) = 1 \\
 &L(q^* q) \geq 0 \quad \text{for all } q \in \mathbb{R}\langle \underline{X} \rangle_{d+1} \\
 &L(h^*(1 - \sum_j X_j^2)h) \geq 0 \quad \text{for all } h \in \mathbb{R}\langle \underline{X} \rangle_d.
 \end{aligned} \tag{(DSDP_{\text{eig-min}})_{d+1}}$$

Proposition 4.4. ($\text{DSDP}_{\text{eig-min}})_{d+1}$ admits Slater points.

Proof. For this it suffices to find a linear map $L : \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$ satisfying $L(p^* p) > 0$ for all nonzero $p \in \mathbb{R}\langle \underline{X} \rangle_{d+1}$, and $L(h^*(1 - \sum_j X_j^2)h) > 0$ for all nonzero $h \in \mathbb{R}\langle \underline{X} \rangle_d$. We again exploit the fact that there are no nonzero polynomial identities that hold for all sizes of matrices, which was used already in Proposition 3.6.

Let us choose $N > d + 1$ and enumerate a dense subset \mathcal{U} of $N \times N$ matrices from \mathbb{B} (for instance, take all $N \times N$ matrices from \mathbb{B} with entries in \mathbb{Q}), that is,

$$\mathcal{U} = \{\underline{A}^{(k)} := (A_1^{(k)}, \dots, A_n^{(k)}) \mid k \in \mathbb{N}, A_j^{(k)} \in \mathbb{B}(N)\}.$$

To each $B \in \mathcal{U}$ we associate the linear map

$$L_B : \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}, \quad f \mapsto \text{tr } f(B).$$

Form

$$L := \sum_{k=1}^{\infty} 2^{-k} \frac{L_{\underline{A}^{(k)}}}{\|L_{\underline{A}^{(k)}}\|}.$$

We claim that L is the desired linear functional.

Obviously, $L(p^* p) \geq 0$ for all $p \in \mathbb{R}\langle \underline{X} \rangle_{d+1}$. Suppose $L(p^* p) = 0$ for some $p \in \mathbb{R}\langle \underline{X} \rangle_{d+1}$. Then $L_{\underline{A}^{(k)}}(p^* p) = 0$ for all $k \in \mathbb{N}$, i.e., for all k we have $\text{tr } p^*(\underline{A}^{(k)})p(\underline{A}^{(k)}) = 0$, hence $p^*(\underline{A}^{(k)})p(\underline{A}^{(k)}) = 0$. Since \mathcal{U} was dense in $\mathbb{B}(N)$, by continuity it follows that $p^* p$ vanishes on all n -tuples from $\mathbb{B}(N)$. Proposition 3.6 implies that $p = 0$. Similarly, $L(h^*(1 - \sum_j X_j^2)h) = 0$ implies $h = 0$ for all $h \in \mathbb{R}\langle \underline{X} \rangle_d$. \blacksquare

Remark 4.5. Having Slater points for $(\text{DSDP}_{\text{eig-min}})_{d+1}$ is important for the clean duality theory of SDP to kick in [VB96, dK02]. In particular, there is no duality gap, so $L_{\text{sohs}} = f_{\text{sohs}} (= f_*)$. Since also the optimal value $f_{\text{sohs}} > -\infty$ (cf. Remark 4.1), f_{sohs} is attained. More important for us and the extraction of optimizers is the fact that L_{sohs} is attained, as we shall explain in §5.

4.3. Optimization of NC polynomials over the polydisc. In this section we consider

$$S = \{1 - X_1^2, \dots, 1 - X_n^2\} \quad (27)$$

and the corresponding nc semialgebraic set

$$\mathbb{D} = \mathcal{D}_S = \bigcup_{k \in \mathbb{N}} \{A = (A_1, \dots, A_n) \in \mathbb{S}_k^n \mid 1 - A_1^2 \succeq 0, \dots, 1 - A_n^2 \succeq 0\},$$

the so-called nc polydisc. Many of the considerations here resemble those from the previous subsection, so we shall be sketchy at times.

The truncated quadratic module tailored for this S is

$$M_{\mathbb{D},d} = \left\{ \sum_i h_i^* s_i h_i \mid h_i \in \mathbb{R}\langle \underline{X} \rangle, s_i \in S \cup \{1\}, \deg(h_i^* s_i h_i) \leq 2d \right\}.$$

Theorem 3.4 implies that the problem $(\text{PSDP}_{\text{eig-min}})$, where S is from (27), yields also the greatest lower bound on the eigenvalues of an nc polynomial f over the polydisc.

Similarly to Proposition 4.2 we can prove:

Proposition 4.6. *Let $f = \sum_{w \in \langle \underline{X} \rangle_{2d}} f_w w$. Then $f \in M_{\mathbb{D},d}$ if and only there exists a positive semidefinite matrix H of order $\sigma(d)$, and positive semidefinite matrices G_i , $1 \leq i \leq n$ of order $\sigma(d-1)$ such that*

$$f_w = \sum_{\substack{u,v \in \langle \underline{X} \rangle_d \\ u^* v = w}} H(u,v) + \sum_i \sum_{\substack{u,v \in \langle \underline{X} \rangle_{d-1} \\ u^* v = w}} G_i(u,v) - \sum_{i=1}^n \sum_{\substack{u,v \in \langle \underline{X} \rangle_{d-1} \\ u^* X_i^2 v = w}} G_i(u,v), \quad \text{for all } w \in \langle \underline{X} \rangle_{2d}. \quad (28)$$

Proof. If $f \in M_{\mathbb{D},d}$ then we can find $h_i \in \mathbb{R}\langle \underline{X} \rangle_d$ and $g_{i,j} \in \mathbb{R}\langle \underline{X} \rangle_{d-1}$ such that

$$f = \sum_i h_i^* h_i + \sum_{i,j} g_{i,j}^* (1 - X_j^2) g_{i,j}.$$

These polynomials yield column vectors H_i and $G_{i,j}$ of length $\sigma(d)$ and $\sigma(d-1)$, respectively, such that $h_i = H_i^t W_d$ and $g_{i,j} = G_{i,j}^t W_{d-1}$. Let us define $H := \sum_i H_i H_i^t$, $G_j := \sum_i G_{i,j} G_{i,j}^t$ and $G := \sum_j G_j$. It follows that

$$\begin{aligned} f &= \sum_i W_d^* H_i H_i^t W_d + \sum_{i,j} W_{d-1}^* G_{i,j} (1 - X_j^2) G_{i,j}^t W_{d-1} \\ &= W_d^* \left(\sum_i H_i H_i^t \right) W_d + W_{d-1}^* \left(\sum_{i,j} G_{i,j} G_{i,j}^t - \sum_j X_j \left(\sum_i G_{i,j} G_{i,j}^t \right) X_j \right) W_{d-1} \\ &= \underbrace{W_d^* H W_d}_{=: S_1} + \underbrace{W_{d-1}^* G W_{d-1}}_{=: S_2} - \underbrace{W_d^* \sum_{i,j} G_i^j (G_i^j)^t W_d}_{=: S_3} \end{aligned}$$

where the column vectors G_i^j are defined by

$$G_i^j(u) = \begin{cases} G_{i,j}(v), & \text{if } u = X_j v, \\ 0, & \text{else.} \end{cases}$$

Let us consider $\tilde{G} := \sum_{i,j} G_i^j (G_i^j)^t$. Suppose $w = u^* v$ for some $u, v \in \langle \underline{X} \rangle_d$. We can find w in S_1 ; the corresponding coefficient is exactly $\sum_{\substack{u,v \in \langle \underline{X} \rangle_d \\ u^* v = w}} H(u, v)$. If we additionally have

$w \in \langle \underline{X} \rangle_{2d-2}$ then w appears also in the summand S_2 with coefficient $\sum_{\substack{u,v \in \langle \underline{X} \rangle_{d-1} \\ u^* v = w}} G(u, v)$. In the

third summand S_3 there appear exactly the words w which can be decomposed as $w = u_1^* X_j^2 v_1$ for some $1 \leq j \leq n$ and some $u_1, v_1 \in \langle \underline{X} \rangle_{d-1}$. Such w have coefficients

$$\begin{aligned} - \sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle \underline{X} \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \tilde{G}(X_j u_1, X_j v_1) &= - \sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle \underline{X} \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \sum_i G_i^j(X_j u_1) G_i^j(X_j v_1) = \\ - \sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle \underline{X} \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} \sum_i G_{i,j}(u_1) G_{i,j}(v_1) &= - \sum_{j=1}^n \sum_{\substack{u_1, v_1 \in \langle \underline{X} \rangle_{d-1} \\ u_1^* X_j^2 v_1 = w}} G_j(u_1, v_1). \end{aligned}$$

Therefore matrices H and G_i are feasible for (28).

To prove the converse we start with rank one decompositions: $H = \sum_i H_i H_i^t$ and $G_j = \sum_i G_{i,j} G_{i,j}^t$. If we define $h_i = H_i^t W_d$ and $g_{i,j} = G_{i,j}^t W_{d-1}$ then feasibility of H and G_j for (28) implies

$$\begin{aligned} \sum_i h_i^* h_i + \sum_{i,j} g_{i,j}^* (1 - X_j^2) g_{i,j} &= \\ \sum_i \sum_{u,v \in W_d} H_i(u) H_i(v) u^* v + \sum_{i,j} \sum_{u,v \in W_{d-1}} \left(G_{i,j}(u) G_{i,j}(v) u^* v - \sum_{i,j} G_{i,j}(u) G_{i,j}(v) u^* X_j^2 v \right) &= \\ = \sum_{w \in W_{2d}} \sum_{\substack{u,v \in W_d \\ u^* v = w}} H(u, v) w + \sum_{w \in W_{2d-2}} \sum_{\substack{u,v \in W_{d-1} \\ u^* v = w}} \sum_j G_j(u, v) w - \sum_{w \in W_{2d}} \sum_j \sum_{\substack{u,v \in W_{d-1} \\ u^* X_j^2 v = w}} G_j(u, v) w &= \\ &= \sum_{w \in W_{2d}} f_w w = f. \quad \blacksquare \end{aligned}$$

Remark 4.7. Similarly to Remark 4.3, the proof of Proposition 4.6 shows how to construct an sohs decomposition with weights (9) for $f \in M_{\mathbb{D},d}$.

By Proposition 4.6, the problem of computing f_* over the polydisc is an SDP. Its dual semidefinite program is:

$$\begin{aligned} L_{\text{sohs}} &= \inf L(f) \\ \text{s. t.} \quad &L : \text{Sym } \mathbb{R} \langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R} \quad \text{is linear} \\ &L(1) = 1 \\ &L(q^* q) \geq 0 \quad \text{for all } q \in \mathbb{R} \langle \underline{X} \rangle_{d+1} \\ &L(h^* (1 - X_j^2) h) \geq 0 \quad \text{for all } h \in \mathbb{R} \langle \underline{X} \rangle_d, 1 \leq j \leq n. \end{aligned}$$

(DSDP_{eig-min})_{d+1}

For implementational purposes, problem $(\text{DSDP}_{\text{eig-min}})_{d+1}$ is more conveniently given as

$$\begin{aligned} L_{\text{sohs}} &= \inf \langle H_L, G_f \rangle \\ \text{s. t.} \quad & H_L(u, v) = H_L(w, z), \text{ if } u^*v = w^*z, \text{ where } u, v, w, z \in \langle \underline{X} \rangle_{d+1} \\ & H_L(1, 1) = 1, H_L \in \mathbb{S}_{\sigma(d+1)}^+, H_L^j \in \mathbb{S}_{\sigma(d)}^+, \forall j \\ & H_L^j(u, v) = H_L(u, v) - H_L(X_j u, X_j v), \text{ for all } u, v \in \langle \underline{X} \rangle_d, 1 \leq j \leq n \end{aligned} \quad (\text{DSDP}'_{\text{eig-min}})_{d+1}$$

where G_f is a Gram matrix for f , and H_L^j represents L acting on nc polynomials of the form $u^*(1 - X_j^2)v$, i.e., H_L^j is the localizing matrix for $1 - X_j^2$.

Proposition 4.8. $(\text{DSDP}_{\text{eig-min}})_{d+1}$ admits Slater points.

Proof. We omit the proof as it is the same as that of Proposition 4.4. ■

Like above, by Proposition 4.8, $L_{\text{sohs}} = f_{\text{sohs}} (= f_*)$ and the optimal value f_{sohs} is attained. Corollary 5.2 from the next section shows that also L_{sohs} is attained.

4.4. Examples. We have implemented the construction of the above SDPs in our open source toolbox [NCS0Stools](#). Using a standard SDP solver (such as SDPA [YFK03], SDPT3 [TTT99] or SeDuMi [Stu99]) the constructed SDPs can be solved. We demonstrate the software on the polynomials from Examples 2.1 and 3.2.

```
>> NCvars x y
>> f1 = 2 + x*y*x*y + y*x*y*x;
>> f2 = 2 - x^2 + x*y^2*x - y^2;
```

We compute the optimal value f_* on the ball by solving $(\text{DSDP}'_{\text{eig-min}})_{d+1}$.

```
>> NCminBall(f1)
ans = 1.5000
>> NCminBall(f2)
ans = 1.0000
```

Similarly we compute f_* on the polydisc by solving $(\text{DSDP}'_{\text{eig-min}})_{d+1}$.

```
>> NCminCube(f1)
ans = 4.0234e-013
>> NCminCube(f2)
ans = 1.0872e-011
```

Note: the minimum of the commutative collapse \check{f}_1 of f_1 over the ball $\mathbb{B}(1) = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 1\}$ and the polydisc $\mathbb{D}(1) = \{(x, y) \in \mathbb{R}^2 \mid |x| \leq 1, |y| \leq 1\}$ is equal to 2 and both minima for \check{f}_2 are equal to 1.

Together with the optimal value f_* our software can also return a certificate for positivity of $f - f_*$, i.e., a sohs decomposition with weights for $f - f_*$ as presented in (8) and (9). For example:

```
>> params.precision=1e-6;
>> [opt,g,decom_sohs,decom_ball] = NCminBall(f2,params)
opt = 1.0000
g = 1-x^2-y^2
decom_sohs = 0
0
```

```

0
0
0
0
y*x
decom_ball = 1
0
0
    
```

yields the following sohs decomposition of the form (8):

$$f_2 - 1 = (y^*x)'*(y^*x) + 1'*(1-x^2-y^2)*1.$$

5. EXTRACT THE OPTIMIZERS

In this section we establish the attainability of f_\star on \mathbb{B} and \mathbb{D} , and explain how to extract the minimizers (\underline{A}, ξ) for f . At the end of the section we present our implementation in [NCSOStools](#).

Proposition 5.1. $f \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$. There exists an n -tuple $\underline{A} \in \mathbb{B}(\sigma(d))$, and a unit vector $\xi \in \mathbb{R}^{\sigma(d)}$ such that

$$f_\star^{\mathbb{B}} = \langle f(\underline{A})\xi, \xi \rangle. \quad (29)$$

In other words, the infimum in (24) is really a minimum. An analogous statement holds for $f_\star^{\mathbb{D}}$.

Proof. By the proof of Theorem 3.4 (or the paragraph on page 6 after the statement of the theorem), $f \succeq 0$ on \mathbb{B} if and only if $f \succeq 0$ on $\mathbb{B}(\sigma(d))$. Thus in (24) we are optimizing

$$(\underline{A}, \xi) \mapsto \langle f(\underline{A})\xi, \xi \rangle \quad (30)$$

over $(\underline{A}, \xi) \in \mathbb{B}(\sigma(d)) \times \{\xi \in \mathbb{R}^{\sigma(d)} \mid \|\xi\| = 1\}$, which is evidently a compact set. Hence by continuity of (30) the infimum is attained. The proof for the corresponding statement for $f_\star^{\mathbb{D}}$ is the same. ■

Corollary 5.2. $f \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$. Then there exists linear functionals

$$L^{\mathbb{B}}, L^{\mathbb{D}} : \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d+2} \rightarrow \mathbb{R}$$

such that $L^{\mathbb{B}}$ is feasible for $(\text{DSDP}_{\text{eig-min}})_{d+1}$, $L^{\mathbb{D}}$ is feasible for $(\text{DSDP}_{\text{eig-min}})_{d+1}$, and we have

$$L^{\mathbb{B}}(f) = f_\star^{\mathbb{B}} \quad \text{and} \quad L^{\mathbb{D}}(f) = f_\star^{\mathbb{D}}. \quad (31)$$

Proof. We prove the statement for $L^{\mathbb{B}}$. Proposition 5.1 implies that there exist \underline{A} and ξ such that $f_\star^{\mathbb{B}} = \langle f(\underline{A})\xi, \xi \rangle$. Let us define $L^{\mathbb{B}}(g) := \langle g(\underline{A})\xi, \xi \rangle$ for $g \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d+2}$. Then $L^{\mathbb{B}}$ is feasible for $(\text{DSDP}_{\text{eig-min}})_{d+1}$ and $L^{\mathbb{B}}(f) = f_\star^{\mathbb{B}}$. The same proof work for $(\text{DSDP}_{\text{eig-min}})_{d+1}$. ■

5.1. Implementation. In this subsection we explain how the optimizers (\underline{A}, ξ) can be extracted from the solutions of the SDPs we constructed in the previous section.

Let $f \in \text{Sym } \mathbb{R}\langle \underline{X} \rangle_{2d}$.

Step 1: Solve $(\text{DSDP}_{\text{eig-min}})_{d+1}$. Let L denote an optimizer, i.e., $L(f) = f_\star$.

Step 2: To L we associate the positive semidefinite matrix $H_L = \begin{bmatrix} H_{\tilde{L}} & B \\ B^t & C \end{bmatrix}$. Modify H_L :

$$H_{\hat{L}} = \begin{bmatrix} H_{\tilde{L}} & B \\ B^t & Z^t H_{\tilde{L}} Z \end{bmatrix},$$

where Z satisfies $H_{\tilde{L}} Z = B$. This matrix yields a flat positive linear map \hat{L} on $\mathbb{R}\langle \underline{X} \rangle_{2d+2}$ satisfying $\hat{L}|_{\mathbb{R}\langle \underline{X} \rangle_{2d}} = L|_{\mathbb{R}\langle \underline{X} \rangle_{2d}}$. In particular, $\hat{L}(f) = L(f) = f_*$.

Step 3: As in the proof of Proposition 3.11, use the GNS construction on \hat{L} to compute symmetric matrices A_i and a unit vector ξ with $\hat{L}(f) = f_* = \langle f(A)\xi, \xi \rangle$.

In Step 3, to construct symmetric matrix representations $A_i \in \mathbb{R}^{\sigma(d) \times \sigma(d)}$ of the multiplication operators we calculate their image according to a chosen basis \mathcal{B} for $E = \text{Ran } H_{\hat{L}}$. To be more specific, $A_i \bar{u}_1$ for $u_1 \in \langle \underline{X} \rangle_d$ being the first label in \mathcal{B} , can be written as a unique linear combination $\sum_{j=1}^s \lambda_j \bar{u}_j$ with words u_j labeling \mathcal{B} such that $L((u_1 X_i - \sum \lambda_j u_j)^*(u_1 X_i - \sum \lambda_j u_j)) = 0$. Then $[\lambda_1 \ \dots \ \lambda_s]^t$ will be the first column of A_i . The vector ξ is the eigenvector of $f(A)$ corresponding to the smallest eigenvalue.

5.2. Examples. We implemented the procedure explained in Steps 1–3 under [NCSOStools](#). Here is a demonstration:

```
>> NCvars x y
>> f2 = 2 - x^2 + x*y^2*x - y^2;

>> [X,fX,eig_val,eig_vec]=NCoptBall(f2)
```

This gives a matrix X of size 2×25 each of whose rows represents one symmetric 5×5 matrix,

$$A = \text{reshape}(X(1, :), 5, 5) = \begin{bmatrix} -0.0000 & 0.7107 & -0.0000 & 0.0000 & 0.0000 \\ 0.7107 & 0.0000 & -0.0000 & 0.3536 & -0.0000 \\ -0.0000 & -0.0000 & -0.0000 & 0.0000 & 0.4946 \\ 0.0000 & 0.3536 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & -0.0000 & 0.4946 & 0.0000 & 0.0000 \end{bmatrix}$$

$$B = \text{reshape}(X(2, :), 5, 5) = \begin{bmatrix} -0.0000 & 0.0000 & 0.7035 & 0.0000 & 0.0000 \\ 0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0000 \\ 0.7035 & 0.0000 & 0.0000 & -0.3588 & 0.0000 \\ 0.0000 & -0.0000 & -0.3588 & 0.0000 & -0.0000 \\ 0.0000 & 0.0000 & 0.0000 & -0.0000 & 0.0000 \end{bmatrix}$$

such that

$$fX = f(A, B) = \begin{bmatrix} 1.0000 & -0.0000 & -0.0000 & 0.0011 & -0.0000 \\ -0.0000 & 1.5091 & -0.0000 & -0.0000 & -0.0000 \\ -0.0000 & -0.0000 & 1.1317 & -0.0000 & -0.0000 \\ 0.0011 & -0.0000 & -0.0000 & 1.7462 & 0.0000 \\ -0.0000 & -0.0000 & -0.0000 & 0.0000 & 1.9080 \end{bmatrix}$$

with eigenvalues $[1.0000, 1.1317, 1.5091, 1.7462, 1.9080]$. So the minimal eigenvalue of $f(A, B)$ is 1 and the corresponding unit eigenvector is $[-1.0000, -0.0000, -0.0000, 0.0015, -0.0000]^t$, when rounded to four digit accuracy.

6. CONCLUDING REMARKS

In this paper we have shown how to effectively compute the smallest (or biggest eigenvalue) a noncommutative (nc) polynomial can attain on the ball \mathbb{B} and the polydisc \mathbb{D} . Our algorithm is based on sums of hermitian squares and yields an exact solution with a *single* semidefinite program (SDP). To prove exactness, we investigated the solution of the dual SDP and used it to extract eigenvalue optimizers with a procedure based on the solution to a *truncated noncommutative moment problem* via flat extensions, and the Gelfand-Naimark-Segal (*GNS construction*). We have also presented the implementation of these procedures in our open source computer algebra system [NCSOStools](http://ncsostools.fis.unm.si/), freely available at <http://ncsostools.fis.unm.si/>.

It is clear that the Nichtnegativstellensatz 3.4 works not only for \mathbb{B} and \mathbb{D} but also for all nc semialgebraic sets obtained from these via invertible linear change of variables. What is less clear (and has been established after we have obtained Theorem 3.4), is that this result can be slightly strengthened. Namely, its conclusion holds for all *convex* nc semialgebraic sets (or, equivalently [HM], nc *LMI domains* \mathcal{D}_L). However, this requires a different and more involved proof. For details we refer the reader to [HKM].

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