Complete Upper Bound Hierarchies for Spectral Minimum in Noncommutative Polynomial Optimization

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Abstract

This work addresses the problem of computing the spectral minimum (ground state energy) of a noncommutative polynomial subject to noncommutative polynomial constraints. Building on the Helton-McCullough Positivstellensatz, the Navascués-Pironio-Acín (NPA) hierarchy provides a sequence of *lower* bounds that converge to the spectral minimum under mild assumptions on the constraint set. Each of these bounds can be computed via semidefinite programming. In this paper, we develop complementary, complete hierarchies of *upper* bounds for the spectral minimum. These are noncommutative counterparts to Lasserre's upper bound hierarchies for classical polynomial optimization. Each upper bound is obtained by solving a generalized eigenvalue problem. The proposed hierarchies are applicable to optimization problems in both bounded and unbounded contexts, as demonstrated through a range of examples.

Contents

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1 Introduction

In this work we consider hierarchies of upper bounds for minimal eigenvalue of noncommutative polynomials over noncommutative *real algebraic sets*, i.e., sets defined by finitely many polynomial equations. Such optimization problems involving multiple operator variables naturally emerge in quantum physics. A notable example is Bell inequalities, originally introduced by [Bel64], which can be interpreted as particular instances of eigenvalue inequalities for noncommutative polynomials (see [PNA10]). In the classical commutative setting, *polynomial optimization* concerns the problem of minimizing a polynomial objective function subject to a finite number of polynomial inequality constraints. As demonstrated, for instance, in [Lau09], this problem is NP-hard to solve exactly. Consequently, numerous approximation techniques have been developed over the past two decades. One prominent example is the *moment-sum of squares* (moment-SOS) hierarchy introduced by [Las01], also known as the Lasserre hierarchy, which is grounded in the Positivstellensatz of Putinar [Put93]. At each level of the hierarchy, a lower bound on the global minimum is obtained by solving a semidefinite program—that is, by minimizing a linear objective function subject to linear matrix inequality constraints (see [VB96]). Under mild assumptions that are often met in practice, such as the presence of a ball constraint, this sequence of lower bounds is guaranteed to converge to the global minimum.

In the noncommutative setting, minimal eigenvalues of noncommutative polynomials can be approximated via a similar hierarchy of lower bounds, known as the Navascués-Pironio-Acín (NPA) hierarchy (see [DLTW08, NPA08, BKP16]), which is based on the noncommutative Positivstellensatz by Helton and McCullough [HM04]. The NPA hierarchy has now become a standard tool in noncommutative optimization and quantum information, and has been extended to tackle a wider range of nonlinear optimization problems; see, e.g., [PKRR+19, KMVW24]. The convergence of this hierarchy is ensured under the same types of assumptions as in the commutative case.

Returning to the commutative setting, an alternative hierarchy proposed in [Las11b] provides a monotonic sequence of *upper* bounds converging to the global minimum of a polynomial over a given set. This hierarchy complements the standard Lasserre lower bound hierarchy. At each step, the corresponding upper bound is computed by solving a *generalized eigenvalue problem*. As with the lower bound hierarchy, the size of the semidefinite variables remains a key factor in determining the scalability of the approach, often limiting direct application to smaller problem instances. To address this for the lower bound hierarchy, researchers have successfully leveraged structural features of input polynomials—such as sparsity and symmetry—to significantly extend its reach; see [MW23] for a recent overview of sparsity-based techniques and [HKP24] for advanced methods applied to Bell inequalities.

A promising direction for improving the efficiency of the upper bound hierarchy was introduced in [Las21], where the focus shifts to the pushforward of the uniform measure under the polynomial of interest. This reformulation transforms the original problem into a univariate optimization task, leading to a new hierarchy of upper bounds constructed from univariate sums of squares of increasing degree. This approach offers computational advantages and new theoretical insights. While certain limitations have been identified in non-compact domains—as recently analyzed in [SW24]—the method represents a significant conceptual advance and opens the door to further developments in bounding techniques.

In contrast to the commutative setting, developing upper bounds for the minimal eigenvalue of noncommutative polynomials remains largely unexplored. Existing results include numerical approaches such as the density matrix renormalization group (DMRG) [Whi92], a variational method developed for capturing the low-energy behavior of quantum many-body systems, quantum variants of Monte Carlo methods [NU98], and convergent approximations for norms in reduced group C^*-algebras [FNT14]. An initial attempt towards a general theory was made in [Ric20], which focused on computing minimal eigenvalues for pure quartic oscillators. However, this approach lacks convergence guarantees and does not scale well to larger problems.

Contributions

The objective of this work is to develop a comprehensive framework for computing upper bounds in noncommutative minimization problems. Specifically, we introduce complete hierarchies of upper bounds for the spectral minimum of noncommutative polynomials within C^*-algebras $\mathcal{A}$, along with corresponding analogues in O^*-algebras of unbounded operators. These hierarchies can be viewed as noncommutative counterparts to those proposed in [Las11b] and [Las21] for the commutative setting.

Analogous to the commutative case, the construction of these hierarchies depends on the choice of a faithful state on $\mathcal{A}$, or more generally, a *separating sequence* of states on $\mathcal{A}$, along with a dense subalgebra of $\mathcal{A}$. In both settings, each upper bound is obtained by solving a single, finite-dimensional generalized eigenvalue problem.

A key factor in the practical applicability of this approach is the computability of the chosen states. While every separable C^*-algebra admits faithful states, these states do not always admit closed-form expressions that are suitable for numerical evaluation. However, in many cases, one can construct separating sequences of states that are effectively computable. One of the advantages of the proposed hierarchies is their ability to accommodate such computable separating sequences.

This framework holds promise for a variety of applications, including estimating spectral minima of polynomial differential operators [Cim10], computing ground state energies of composite Hamiltonians in mathematical physics [AGN24], and quantifying violations of probabilistic inequalities in quantum information theory [PKRR$^+$19]. For instance, it can be directly applied to approximate violations of Bell inequalities by employing tensor products of universal group C^*-algebras equipped with separating state sequences. These can be evaluated using techniques such as Haar integration over unitary groups (see [CS06]).

Additionally, we demonstrate the applicability of our approach on examples involving polynomial differential operators using the faithful vector state induced by the standard multivariate Gaussian, as well as on analytic (non-polynomial) functions in operator variables. For each of these cases, we provide heuristic estimates for the convergence rates of the proposed hierarchies.

The present paper supersedes the earlier extended abstract [KMMV24] presented at the MTNS conference in 2024, which contained incorrect results. We now outline how our present contributions compare to that previous short preliminary announcement, explain the source of those errors, and present the corrected results:

1. In [KMMV24] preliminary hierarchies of upper bounds have been derived for separable C^*-algebras, based on the notion of increasing separable state sequences. It turns out that the main result from [KMMV24, Theorem 1] provided a wrong characterization of positive elements by means of such increasing sequences; see Remark 4 below. Therefore the convergence result from [KMMV24, Corollary 2] also turns out to be wrong. The current article proposes in Theorem 3 a corrected characterization of positivity, based on sequences converging to faithful states. Thanks to this characterization, the convergence of the hierarchy of upper bounds is proved in Section 3.4. Furthermore, crucially this article extends the framework also to unbounded operator algebras (O^*-algebras).

2. A methodology to obtain a hierarchy of lower bounds for maximal violation levels for Bell inequalities was presented in [KMMV24, Section 3.2], yet without proofs. In order to formally justify this methodology, we state and prove the required theoretical result in Proposition 14.

3. Moreover, numerical examples of various other spectral minimum problems are given, including those with a non-polynomial objective function or unbounded operator domain.

Acknowledgments

2 Commutative inspiration

We start by recalling a few useful results in the commutative case. The support of a Borel measure μ on $\mathbb{R}^n$, denoted by $\operatorname{supp}\mu$, is the (unique) smallest closed set $\mathbf{X}$ such that $\mu(\mathbb{R}^n\backslash\mathbf{X}) = 0$. Given a Borel measure μ with $\operatorname{supp}\mu = \mathbf{X}$, let $\mathbf{z} = (z_\alpha)_{\alpha\in\mathbb{N}^n}$ be a real sequence whose entries are the moments of μ, called its *moment sequence*, i.e., $z_\alpha = \int_{\mathbf{X}} x^\alpha \mathrm{d}\mu(x)$, for all $\alpha \in \mathbb{N}^n$. Let $\mathbb{R}[x]$ be the vector space of commutative polynomials.

For a given sequence $\mathbf{z} \in \mathbb{R}^{\mathbb{N}^n}$ we introduce the Riesz linear functional

$$L_{\mathbf{z}} : \mathbb{R}[x] \to \mathbb{R}$$

$$f\left(= \sum_{\alpha\in\mathbb{N}^n} f_\alpha x^\alpha\right) \mapsto L_{\mathbf{z}}(f) = \sum_{\alpha\in\mathbb{N}^n} f_\alpha z_\alpha. \tag{1}$$

With $d \in \mathbb{N}$, the truncated commutative multivariate *Hankel matrix* $\mathbf{M}_d(\mathbf{z})$ associated with $\mathbf{z}$ is the real symmetric matrix with rows and columns indexed by the canonical basis (x^α) and with entries:

$$\mathbf{M}_d(\mathbf{z})(\alpha,\beta) := L_{\mathbf{z}}(x^{\alpha+\beta}) = z_{\alpha+\beta}, \quad \alpha,\beta \in \mathbb{N}^n_d,$$

where $\mathbb{N}^n_d := \{\alpha \in \mathbb{N}^n \mid \alpha_i \le d,\ i = 1,\ldots,n\}$. This matrix is the multivariate version of a (univariate) Hankel matrix.

Similarly, for all $f \in \mathbb{R}[x]$, the truncated *localizing matrix* $\mathbf{M}_d(f\,\mathbf{z})$ associated with $\mathbf{z}$ and f is the real symmetric matrix with rows and columns indexed by the canonical basis (x^α) and with entries:

$$\mathbf{M}_d(f\,\mathbf{z})(\alpha,\beta) := L_{\mathbf{z}}(f\,x^{\alpha+\beta}) = \sum_\gamma f_\gamma z_{\alpha+\beta+\gamma}, \quad \alpha,\beta \in \mathbb{N}^n_d.$$

The localizing matrix associated to $f = 1$ corresponds to the above-defined multivariate Hankel matrix.

Let us recall a key preliminary result provided in [Las11b, Theorem 3.2].

Theorem 1. *Let $\mathbf{X}$ be compact and μ be a Borel measure with moment sequence $\mathbf{z}$ and $\operatorname{supp}\mu = \mathbf{X}$. Then a polynomial f is nonnegative on $\mathbf{X}$ if and only if $\mathbf{M}_d(f\,\mathbf{z}) \succeq 0$ for all $d \in \mathbb{N}$.*

The result from Theorem 1 is actually valid for every continuous function f, thus in a quite general context, by considering a localizing matrix with entries being $\int_{\mathbf{X}} f(x) x^{\alpha+\beta} \mathrm{d}\mu(x)$, $\alpha,\beta \in \mathbb{N}^n_d$. In the polynomial case, it can be concretely applied when the moments of μ are readily available, for instance when $\mathbf{X}$ is the unit ball/box, and μ is the restriction of the Lebesgue measure on $\mathbf{X}$.

Now, let us fix an arbitrary Borel measure μ with moment sequence $\mathbf{z}$ and $\operatorname{supp}\mu = \mathbf{X}$, and consider the problem of computing the minimum $\sigma_{\min}(f)$ of a commutative polynomial f over the compact set $\mathbf{X}$. Invoking Theorem 1, in [Las11b] Lasserre provides a monotone sequence of upper bounds converging to $\sigma_{\min}(f)$, by solving the hierarchy of semidefinite programs indexed by $d \in \mathbb{N}$:

$$\begin{aligned} \lambda_d = \sup_{\lambda\in\mathbb{R}} \quad & \lambda \\ \text{s.t.} \quad & \mathbf{M}_d(f\,\mathbf{z}) \succeq \lambda\,\mathbf{M}_d(\mathbf{z}). \end{aligned} \tag{2}$$

Since $\ker \mathbf{M}_d(f\,\mathbf{z}) \supseteq \ker \mathbf{M}_d(\mathbf{z})$ by the Cauchy-Schwarz inequality, (2) reduces to a generalized eigenvalue problem (i.e., by projecting onto the complement of $\ker \mathbf{M}_d(\mathbf{z})$ one obtains a version of (2) with a positive definite matrix on the right), for which efficient standard linear algebra routines exist.

Theorem 2 ([Las11b, Theorem 4.1]). *Let $\mathbf{X} \subseteq \mathbb{R}^n$ be a compact set, μ be a Borel measure with moment sequence $\mathbf{z}$ and $\operatorname{supp} \mu = \mathbf{X}$, and $f \in \mathbb{R}[x]$. Consider the hierarchy of semidefinite programs (2) indexed by $d \in \mathbb{N}$. Then:*

(a) *The problem (2) has an optimal solution $\lambda_d \geq \sigma_{\min}(f)$ for every $d \in \mathbb{N}$;*

(b) *The sequence $(\lambda_d)_{d \in \mathbb{N}}$ is monotone nonincreasing and $\lambda_d \downarrow \sigma_{\min}(f)$ as $d \to \infty$.*

More recently, in [Las21] it has been shown that $\sigma_{\min}(f)$ can also be approximated from above by considering a hierarchy of generalized eigenvalue problems indexed by d, but now involving Hankel matrices of size $d+1$ instead of $\binom{n+d}{n}$. The entries of these matrices are linear in the moments of the *pushforward measure* of the Lebesgue measure with respect to f.

Pushforward measure. Given compact sets $\mathbf{X}$ and $\boldsymbol{\Omega}$, let $f : \mathbf{X} \to \boldsymbol{\Omega} \subseteq \mathbb{R}$ be a continuous function, and μ be a Borel measure with $\operatorname{supp} \mu = \mathbf{X}$. The *pushforward measure $f_{\#}\mu$* of the measure μ through f is defined by

$$f_{\#}\mu(C) = \mu(f^{-1}(C)), \tag{3}$$

for any C in the Borel algebra of Ω, and $f^{-1}(C)$ is the preimage of C by the mapping f.

The moment sequence of $f_{\#}\mu$ is denoted by $\mathbf{z}^{\#} = (z_d^{\#})_{d \in \mathbb{N}}$ and given by

$$z_d^{\#} := \int_{\mathbb{R}} u^d \, \mathrm{d}f_{\#}\mu(u) = \int_{\mathbf{X}} f(x)^d \mathrm{d}\mu(x) = L_{\mathbf{z}}(f^d).$$

Let us define

$$\mathbf{M}_{k,d}(f\,\mathbf{z}) := \left(L_{\mathbf{z}}(f^{i+j+k}) \right)_{i,j=0}^{d} = (z_{i+j+k}^{\#})_{i,j=0}^{d}.$$

As in [Las21], let us consider the hierarchy of generalized eigenvalue problems, indexed by $d \in \mathbb{N}$:

$$\begin{aligned} \eta_d = \sup_{\eta \in \mathbb{R}} \quad & \eta \\ \text{s.t.} \quad & \mathbf{M}_{1,d}(f\,\mathbf{z}) \succeq \eta \, \mathbf{M}_{0,d}(f\,\mathbf{z}). \end{aligned} \tag{4}$$

Since the support of $f_{\#}\mu$ is contained in the interval $[\sigma_{\min}(f), +\infty)$, the results from [Las11a, Theorem 3.3] imply that η_d is attained for all $d \in \mathbb{N}$ and $\eta_d \downarrow \sigma_{\min}(f)$ as $d \to \infty$ (see also [Las21, Theorem 2.3]).

3 Upper bounds for spectral minimum

We state our optimization problem in a similar way as in [KMMV24]. Let F be a noncommutative polynomial in m variables. We are concerned with problems involving either the optimization or the verification of positive semidefiniteness of the evaluation $F(X_1, \ldots, X_m)$, where $(X_1, \ldots, X_m)$ ranges over tuples of operators subject to prescribed polynomial constraints. Such operator tuples often arise as representations of a single (typically infinite-dimensional) algebra $\mathcal{A}$, in which case the positivity of F evaluated on these operators corresponds to the positivity of a single element $f \in \mathcal{A}$.

For instance, consider the question of whether $F(U_1, \ldots, U_n)$ is positive semidefinite for all tuples $(U_1, \ldots, U_n)$ of unitary operators acting on a separable Hilbert space. This problem is equivalent to asking whether the element $f = F(W_1, \ldots, W_n)$ is positive in the universal group C^*-algebra $C^*(\mathbb{Z}^{\star n})$, where $W_1, \ldots, W_n$ denote the canonical unitary generators.

Accordingly, our approach to positivity and eigenvalue optimization is formulated in terms of the positivity of elements within operator algebras. We first address optimization in bounded operator variables, and thus start by recalling some necessary background on C^*-algebras.

3.1 C^*-algebra basics

We refer to [Tak02, Chapter I] for a comprehensive introduction to C^*-algebras. A C^*-*algebra* $\mathcal{A}$ is a complex algebra endowed with an involution $*$ and a norm $\|\cdot\|$, such that $\mathcal{A}$ is a complete normed space, and the norm is sub-multiplicative ($\|ab\| \leq \|a\|\|b\|$) and satisfies the C^*-identity $\|a^*a\| = \|a\|^2$. Equivalently [Tak02, Theorem 9.18], $\mathcal{A}$ is an algebra of bounded operators on a Hilbert space that is closed in norm topology and closed under taking adjoints. In this article, all C^*-algebras are assumed to be unital (containing the multiplicative identity 1). A $*$-representation π of $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is a $*$-homomorphism $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ (this definition is valid for a general complex algebra with involution $\mathcal{A}$).

Let us mention some standard constructions that we will refer to later. There are two natural ways of associating a C^*-algebra with a discrete group G. The reduced C^*-algebra $\mathrm{C}^*_{\mathrm{red}}(G)$ is the operator norm completion of the group ring $\mathbb{C}[G]$ acting on the Hilbert space $L^2(G)$ by left multiplication. The full C^*-algebra $\mathrm{C}^*_{\mathrm{full}}(G)$ is the completion of the group ring $\mathbb{C}[G]$ with respect to the norm $\|a\| = \sup_\rho \|\rho(a)\|$ over all unitary representations ρ of G. In general, $\mathrm{C}^*_{\mathrm{red}}(G)$ is a quotient of $\mathrm{C}^*_{\mathrm{full}}(G)$. Similarly, there are two natural ways of completing the algebraic tensor product $\mathcal{A}_1 \otimes \mathcal{A}_2$ to a C^*-algebra. Its completion with respect to the norm $\|a\| = \sup_{\pi_1, \pi_2} \|(\pi_1 \otimes \pi_2)(a)\|$ over all $*$-representations π_j of $\mathcal{A}_j$ is called the minimal tensor product and denoted $\mathcal{A}_1 \otimes_{\min} \mathcal{A}_2$. Its completion with respect to the norm $\|a\| = \sup_\pi \|\pi(a)\|$ over all $*$-representations π of $\mathcal{A}_1 \otimes \mathcal{A}_2$ is called the maximal tensor product and denoted $\mathcal{A}_1 \otimes_{\max} \mathcal{A}_2$. In general, $\mathcal{A}_1 \otimes_{\min} \mathcal{A}_2$ is a quotient of $\mathcal{A}_1 \otimes_{\max} \mathcal{A}_2$.

Let $\mathcal{A}$ be a C^* algebra. The *spectrum* of $a \in \mathcal{A}$ is $\sigma(a) = \{\lambda \in \mathbb{C} \colon a - \lambda 1 \text{ not invertible in } \mathcal{A}\}$, and is a compact nonempty set in $\mathbb{C}$. A self-adjoint element $a = a^* \in \mathcal{A}$ has spectrum contained in $\mathbb{R}$, and is *positive semidefinite* if its spectrum is contained in $\mathbb{R}_{\geq 0}$; or equivalently [Tak02, Theorem 6.1], $a = b^*b$ for some $b \in \mathcal{A}$. A *state* on a C^*-algebra $\mathcal{A}$ is a unital positive linear functional $\phi : \mathcal{A} \to \mathbb{C}$ (that is, $\phi(1) = 1$ and $\phi(a^*a) \geq 0$ for $a \in \mathcal{A}$). A state ϕ on $\mathcal{A}$ is called *faithful* if $\phi(a^*a) = 0$ implies $a = 0$ for all $a \in \mathcal{A}$. A sequence of states $(\phi_d)_d$ on $\mathcal{A}$ is called *separating* if for every nonzero $a \in \mathcal{A}$ there exists $d \in \mathbb{N}$ such that $\phi_d(a^*a) > 0$. If $(\phi_d)_d$ is a separating sequence on $\mathcal{A}$, and

$$\tilde{\phi}_d = \frac{2^d}{2^d - 1} \sum_{i=1}^{d} \frac{1}{2^i} \phi_i, \tag{5}$$

then $(\tilde{\phi}_d)_d$ converges in the weak-$*$ (pointwise) topology to a faithful state on $\mathcal{A}$. It is well-known that separable C^*-algebras, including finitely generated C^*-algebras, always admit faithful states [Tak02, Exercise I.9.3].

Our goal is to approximate from above the minimum of the spectrum of a self-adjoint $f \in \mathcal{A}^*$, i.e.,

$$\sigma_{\min}(f) := \min \sigma(f) = \sup\{\alpha \in \mathbb{R} \colon f - \alpha 1 \succeq 0\}.$$

Note that this minimum exists since $\sigma(f)$ is compact and nonempty. The spectral minimum $\sigma_{\min}(f)$, also called the ground state energy of f, is in general smaller than the lowest eigenvalue of f. For example, $f \in \mathcal{A} = L^\infty([0,1])$ acting on $L^2([0,1])$ as $f(g)(t) = tg(t)$ has no eigenvalues, yet $\sigma(f) = [0,1]$, and so $\sigma_{\min}(f) = 0$.

3.2 Positivity in C^*-algebras via faithful functionals

Let $\mathcal{A}$ be a C^*-algebra. For a given subset $S \subset \mathcal{A}$, the $*$-words in S are the products of elements of S and their adjoints. We denote by $\mathbb{C}\langle S \rangle_d$ the span of all $*$-words in S of length at most d, and by $\mathbb{C}\langle S \rangle$ the $*$-algebra generated by S. That is, elements of $\mathbb{C}\langle S \rangle$ are noncommutative polynomials in elements of S and their adjoints. A set $S \subset \mathcal{A}$ is called *generating* if $\mathcal{A}$ is the closure in the norm topology of $\mathbb{C}\langle S \rangle$. The following is a C^*-algebraic (noncommutative bounded) analog of Theorems 1 and 2.

Theorem 3. *Let $\mathcal{A}$ be a C^*-algebra, S its generating set, and $(\phi_d)_d$ a sequence of states on $\mathcal{A}$ converging to a faithful state ϕ. For $f = f^* \in \mathcal{A}$, the following are equivalent:*

(i) $f \succeq 0$ in $\mathcal{A}$;

(ii) $\phi(h^* f h) \geq 0$ for all $h \in \mathbb{C}\langle S \rangle$;

(iii) for every $d \in \mathbb{N}$, $\phi_d(h^* f h) \geq 0$ for all $h \in \mathbb{C}\langle S \rangle_d$;

(iv) $\phi(p(f)^2 f) \geq 0$ for all $p \in \mathbb{R}[t]$;

(v) for every $d \in \mathbb{N}$, $\phi_d(p(f)^2 f) \geq 0$ for all $p \in \mathbb{R}[t]_d$.

Proof. The implications (i)$\Rightarrow$(ii)-(v) are clear.

(ii)$\Rightarrow$(i): Since S is generating and ϕ is continuous in norm topology, we have $\phi(a^* f a) \geq 0$ for all $a \in \mathcal{A}$. Let $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ be the cyclic $*$-representation of $\mathcal{A}$ induced by ϕ by the Gelfand-Naimark-Segal (GNS) construction [Tak02, Theorem 9.14]. That is, there is a unit vector $v \in \mathcal{H}$ such that $\pi(\mathcal{A})v$ is dense in $\mathcal{H}$, and $\phi(a) = \langle \pi(a)v, v \rangle$ for all $a \in \mathcal{A}$. Then π is a $*$-embedding since ϕ is faithful, and $\pi(f) \succeq 0$ in $\mathcal{B}(\mathcal{H})$. Therefore $f \succeq 0$ in $\mathcal{A}$ by [Tak02, Proposition I.4.8 and Theorem I.6.1].

(iii)$\Rightarrow$(ii): Let $h \in \mathbb{C}\langle S \rangle$ be arbitrary, and let $d_0 \in \mathbb{N}$ be such that $h \in \mathbb{C}\langle S \rangle_{d_0}$. Then $\phi_d(h^* f h) \geq 0$ for all $d \geq d_0$. Since $(\phi_d)_d$ converges to ϕ, we have $\phi(h^* f h) \geq 0$.

(v)$\Rightarrow$(iv): The argument is analogous to (iii)$\Rightarrow$(ii).

(iv)$\Rightarrow$(i): Let $\mathcal{B}$ be the abelian C^*-subalgebra in $\mathcal{A}$ generated by f. By the proof (ii)$\Rightarrow$(i) (with $\mathcal{B}$ and $\{f\}$ in place of $\mathcal{A}$ and S, respectively), $f \succeq 0$ in $\mathcal{B}$. Therefore, $f = b^* b$ for some $b \in \mathcal{B}$, so $f \succeq 0$ in $\mathcal{A}$. ∎

Remark 4. The precursor of Theorem 3 in [KMMV24] is false. Therein, [KMMV24, Theorem 1] asserted the conclusion of Theorem 3 based on a weaker assumption that $(\phi_d)_d$ is an increasing separating sequence of states on $\mathcal{A}$ (that does not necessarily converge to a faithful state). Here, increasing means that for every d there is $\alpha > 0$ such that $\phi_d(a^* a) \leq \alpha \phi_{d+1}(a^* a)$ for all $a \in \mathcal{A}$. However, this is not sufficient, as we now demonstrate.

Let $\mathcal{A} = \mathcal{C}[-1, 1]$ be the commutative C^*-algebra of continuous functions on $[-1, 1]$. Then, $\psi(a) = \frac{1}{2} \int_{-1}^{1} a(t) \, dt$ and $\phi(a) = 2 \int_{1/2}^{1} a(t) \, dt$ are states on $\mathcal{A}$, and ψ is faithful. For every $d \in \mathbb{N}$, there exists $\varepsilon_d > 0$ such that $\phi(p^2 t) \geq \varepsilon_d \|p\|^2$ for all $p \in \mathbb{C}[t]_d$ (because $t \geq \frac{1}{2}$ on $[\frac{1}{2}, 1]$, and $\mathbb{C}[t]_d$ is a finite-dimensional space). Without loss of generality we can assume that $(\varepsilon_d)_d$ is decreasing. Define $\phi_d := \frac{1}{1+\varepsilon_d} \phi + \frac{\varepsilon_d}{1+\varepsilon_d} \psi$. Then, ϕ_d is a faithful state on $\mathcal{A}$, and

$$\phi_d(a^* a) \leq \frac{\varepsilon_d}{\varepsilon_{d+1}} \cdot \frac{1}{1+\varepsilon_d} \phi(a^* a) + \frac{\varepsilon_d}{1+\varepsilon_d} \psi(a^* a) = \frac{\varepsilon_d(1+\varepsilon_{d+1})}{\varepsilon_{d+1}(1+\varepsilon_d)} \cdot \phi_{d+1}(a^* a)$$

for all $a \in \mathcal{A}$. Let us compare assertions (i) and (iii) in Theorem 3 for $(\phi_d)_d$, $S = \{t\}$ and $f(t) = t$. On the one hand, $f \not\succeq 0$ in $\mathcal{A}$. On the other hand, for every $d \in \mathbb{N}$,

$$\phi_d(p^2 f) = \frac{1}{1+\varepsilon_d} \phi(p^2 t) + \frac{\varepsilon_d}{1+\varepsilon_d} \psi(p^2 t) \geq \frac{1}{1+\varepsilon_d} \varepsilon_d \|p\|^2 - \frac{\varepsilon_d}{1+\varepsilon_d} \|p\|^2 \geq 0$$

for all $p \in \mathbb{C}[t]_d$. Note that while $(\phi_d)_d$ converges to ϕ, the latter is not faithful.

Example 5. We recall some well-known separable C^*-algebras together with their faithful states, or separating sequences of states, which give rise to sequences converging to faithful states as in (5). With the exception of (b), all have been already mentioned in [KMMV24, Section 3.1].

(a) Let G be a finitely generated discrete group. Then the canonical tracial state τ on the reduced C^*-algebra $C^*_{\mathrm{red}}(G)$, determined on G by

$$\tau(g) = \begin{cases} 1 & \text{if } g = \mathrm{id}, \\ 0 & \text{otherwise}, \end{cases}$$

is faithful.

(b) Let Γ be a finite directed graph with vertices V, edges E, and source and range maps $r, s :$ $E \to V$ denoting the endpoints of the edges. The graph C^* algebra of Γ is generated by mutually orthogonal projections (denoted by vertices in V) and partial isometries with mutually orthogonal ranges (denoted by edges in E) with defining relations $e^*e = r(e)$ for all $e \in E$ and $\sum_{s(e)=v} ee^* = v$ for all $v \in V$. For example, the Cuntz algebra and the Toeplitz algebra are examples of such algebras. The graph C^*-algebra of Γ admits a faithful state that is evaluated in terms of paths and vertex degrees in the graph Γ [AG11, Theorem 2.1].

(c) The full C^*-algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ admits a separating sequence

$$\phi_d(w) = \frac{1}{d} \int_{U \in \mathrm{U}_d(\mathbb{C})^n} \mathrm{tr}\, w(U)\, \mathrm{d}U. \tag{6}$$

The separating property of (6) is a consequence of [Cho80, Theorem 7] (see [KVV17, Corollary 4.7] for more details). Via (5), the states ϕ_d give rise to a sequence converging to a faithful state on $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. Note that when restricted to $\mathbb{C}[\mathbb{Z}^{\star n}]$, the sequence $(\phi_d)_d$ itself converges to the canonical tracial state τ on $\mathbb{C}[\mathbb{Z}^{\star n}]$ [Voi91, Theorem 3.8], which leads to the C^*-algebra $\mathrm{C}^*_{\mathrm{red}}(\mathbb{Z}^{\star n})$; thus, (5) is required when working with $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. As already explained in [KMMV24], one can efficiently evaluate the states (6) by means of the Collins-Śniady calculus for Haar integration over unitary groups [CS06, Corollary 2.4].

(d) Let us consider two C^*-algebras $\mathcal{A}_1$ and $\mathcal{A}_2$ with faithful states ϕ_1 and ϕ_2, respectively. As a consequence of [Tak02, Theorem IV.4.9], the state $\phi_1 \otimes \phi_2$ on the minimal tensor product $\mathcal{A}_1 \otimes_{\mathrm{min}} \mathcal{A}_2$ is faithful. As a consequence of [Dyk98, Theorem 1.1], the state $\phi_1 \star \phi_2$ on the reduced free product $\mathcal{A}_1 \star \mathcal{A}_2$ is faithful. One can easily evaluate $\phi_1 \otimes \phi_2$ and $\phi_1 \star \phi_2$ using the values of ϕ_1 and ϕ_2.

(e) One can combine (c) and (d) to obtain an explicit separating sequence for the algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\mathrm{min}} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. We refer to Section 4 for more details. We emphasize that $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\mathrm{min}} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ is not isomorphic in general to $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\mathrm{max}} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n}) \cong \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m} \times \mathbb{Z}^{\star n})$ for $m, n > 2$ as a consequence of the refutation [JNV+21] of Connes' embedding conjecture [Con76, KS08] and its equivalent Kirchberg conjecture [Kir93, Oza13].

In the case of discrete groups, let us comment on the distinction between the full and reduced C^*-algebra, from a positivity perspective.

Remark 6. Let G be the free group on n generators $S = \{g_1, \ldots, g_n\}$. By [KVV17, Corollary 4.13] (see also [HMP04, Section 4.2]), the following are equivalent for $f \in \mathbb{C}\langle S \rangle_d$:

(i) $f \succeq 0$ in $\mathrm{C}^*_{\mathrm{full}}(G)$;

(ii) $f \succeq 0$ on $\mathrm{U}_K(\mathbb{C})^n$, where $K = (2n+1)^{d+1}$;

(iii) $f = \sum_i h_i^* h_i$ for $h_i \in \mathbb{C}\langle S \rangle_{d+1}$.

These conditions are in general strictly stronger than $f \succeq 0$ in $\mathrm{C}^*_{\mathrm{red}}(G)$ if $n \geq 2$. For example, let $f = \frac{\sqrt{2n-1}}{n} - \frac{1}{2n} \sum_{i=1}^n (g_i + g_i^{-1})$. Then $f \succeq 0$ in $\mathrm{C}^*_{\mathrm{red}}(G)$ by [Kes59b, Theorem 3], but f is negative under the homomorphism induced by the trivial representation of G when $n \geq 2$, namely $f(1, \ldots, 1) = \frac{\sqrt{2n-1}}{n} - 1 < 0$.

More generally, let G be a discrete group generated by n generators $g_1, \ldots, g_n$, and let $m = \frac{1}{2n} \sum_{i=1}^n (g_i + g_i^{-1})$. Then $1 - m - \varepsilon$ is negative under the trivial representation of G for every $\varepsilon > 0$; on the other hand, $1 - m - \varepsilon \succeq 0$ in $\mathrm{C}^*_{\mathrm{red}}(G)$ for some $\varepsilon > 0$ if and only if G is not amenable by [Kes59a, §3 Theorem].

3.3 Positivity in O^*-algebras

Let us record an observation for unbounded operator algebras in the spirit of Theorem 3. In contrast with the bounded context of Section 3.2, positivity on unbounded domains can rarely be characterized using sums of hermitian squares (exceptions are, for example, positivity subject to linear matrix inequalities [HKM12] or in Weyl algebras [Sch05]). Consequently, results on noncommutative optimization on unbounded domains are sporadic. Thus, the following formalism (and its consequence for optimization in Section 3.4) is virtually the sole general approach to optimization in unbounded operator variables.

Since working with unbounded operators brings along certain subtleties, we first introduce some suitable auxiliary terminology [Sch90]. Let $\mathcal{H}$ be a complex Hilbert space, and $\mathcal{D}$ its dense subspace. A set $\mathcal{O}$ of closable operators $\mathcal{D} \to \mathcal{H}$ is an O^*-*algebra on $\mathcal{H}$ with domain $\mathcal{D}$* [Sch90, Definition 2.1.6] if $\mathcal{O}$ contains the scalar multiples of the identity on $\mathcal{D}$, $a\mathcal{D} \subseteq \mathcal{D}$ for all $a \in \mathcal{O}$, $\mathcal{O}$ is closed under addition and multiplication, and for every $a \in \mathcal{O}$, its adjoint a^* on $\mathcal{H}$ is defined on $\mathcal{D}$ and $a^\star := a^*|_{\mathcal{D}} \in \mathcal{O}$. Furthermore, $\mathcal{O}$ is *closed* [Sch90, Definition 2.2.8] if its domain $\mathcal{D}$ is complete in the *graph topology* of $\mathcal{O}$ (the locally convex topology defined by seminorms $\{v \mapsto \|av\| \colon a \in \mathcal{O}\}$). A vector $u \in \mathcal{D}$ is *cyclic* for $\mathcal{O}$ if $\mathcal{O} \cdot u$ is dense in $\mathcal{D}$ with respect to the graph topology of $\mathcal{O}$; then $\phi : \mathcal{O} \to \mathbb{C}$ given as $\phi(a) = \frac{1}{\|u\|^2} \langle au, u \rangle$ is called a *faithful vector state* on $\mathcal{O}$.

An operator f in an O^*-algebra $\mathcal{O}$ with domain $\mathcal{D}$ is positive semidefinite if $\langle fv, v \rangle \geq 0$ for all $v \in \mathcal{D}$. If $u \in \mathcal{D}$ is a cyclic vector for $\mathcal{O}$, denseness in the graph topology implies that for checking $f \succeq 0$, it suffices to restrict to $v \in \mathcal{O} \cdot u$. A consequence of these setup and observation is the following.

Corollary 7. *Let $\mathcal{O}$ be a closed O^*-algebra, and ϕ a faithful vector state on $\mathcal{O}$. For $f = f^\star \in \mathcal{O}$, the following are equivalent:*

(i) *$f \succeq 0$ in $\mathcal{O}$;*

(ii) *$\phi(h^\star f h) \geq 0$ for all $h \in \mathcal{O}$.*

Corollary 7 is weaker than Theorem 3 in several aspects. While Theorem 3 addresses positive semidefiniteness in all $*$-representations of a C^*-algebra, Corollary 7 essentially only addresses positive semidefiniteness in one representation (namely, the concrete given realization of the O^*-algebra, and not in its other representations). Next, while every positive semidefinite element of a C^*-algebra is a hermitian square, and every unital linear functional strictly positive on nonzero hermitian squares is a faithful state, the analogs of these conclusions for O^*-algebras fail (hence the more restricted setup for Corollary 7 is required). Finally, Corollary 7 does not admit a part (iv) as in Theorem 3. In fact, a direct unbounded analog of Theorem 3 fails. This is shown in [SW24] in the commutative setting, and we present a streamlined self-contained example in Subsection 3.3.1 below.

The following are some important examples of closed O^*-algebras and their cyclic vector states.

Example 8. Consider the Weyl algebra $\mathcal{W} = \mathbb{C}\langle x, y \colon xy - yx = 1 \rangle$ with $x^\star = -x$ and $y^\star = y$. It arises naturally in the context of Heisenberg's uncertainty principle and canonical quantization, and abstracts the momentum (differential) and position (multiplication) operators. By the Stone-von Neumann theorem [RS80, Theorem VIII.14], $\mathcal{W}$ has a unique representation as an O^*-algebra, as follows. The Schrödinger representation of $\mathcal{W}$ [Sch90, Example 2.5.2] on $L^2(\mathbb{R})$ is the O^*-algebra $\mathcal{O}$ with domain $\mathcal{S}(\mathbb{R})$, the Schwartz space of rapidly decreasing functions, generated by operators X, Y defined as $Xs = \frac{d}{dt}s$ and $Ys = ts$ for $s \in \mathcal{S}(\mathbb{R})$ (and the closures of iX and Y are self-adjoint operators). The unit vector $u = \frac{1}{\sqrt[4]{\pi}} e^{-\frac{t^2}{2}} \in \mathcal{S}(\mathbb{R})$ is cyclic for $\mathcal{O}$ by [Sch90, Example 8.6.15]. Let ϕ be the faithful vector state induced by u; let us view ϕ as a functional on $\mathcal{W}$ (by identifying x, y with X, Y). Note that $\mathcal{W} = \mathbb{C}\langle a, a^\star \colon aa^\star - a^\star a = 1 \rangle$ where $a = \frac{x+y}{\sqrt{2}}$ (the Fock-Bargmann representation of $\mathcal{W}$ [Fol89,

Section 1.6]). On the basis $\{a^{*m}a^n : m, n \in \{0\} \cup \mathbb{N}\}$ for $\mathcal{W}$, the faithful vector state ϕ is then given as

$$\phi(a^{\star m}a^n) = \left\langle \left(\frac{-X+Y}{\sqrt{2}}\right)^m \left(\frac{X+Y}{\sqrt{2}}\right)^n u, u \right\rangle = \sqrt{2}^{-m-n} \int_{\mathbb{R}} \left(\left(\tfrac{\mathrm{d}}{\mathrm{d}t} + t\right)^m u\right) \left(\left(\tfrac{\mathrm{d}}{\mathrm{d}t} + t\right)^n u\right) \, \mathrm{d}t$$

$$= \begin{cases} 1 & \text{if } m = n = 0, \\ 0 & \text{otherwise.} \end{cases}$$

By Corollary 7, $f(X, Y)$ acting on $\mathcal{S}(\mathbb{R})$ is positive semidefinite if and only if $\phi(h^\star fh) \geq 0$ for all $h \in \mathcal{W}$.

More generally, the same reasoning applies to the nth Weyl algebra $\mathcal{W}^{\otimes n}$, whose representation on $L^2(\mathbb{R}^n)$ with domain $\mathcal{S}(\mathbb{R}^n)$ is generated by differential operators $\frac{\mathrm{d}}{\mathrm{d}t_1}, \ldots, \frac{\mathrm{d}}{\mathrm{d}t_n}$ and multiplication operators $t_1, \ldots, t_n$. Its cyclic unit vector is $\pi^{-\frac{n}{4}} e^{-\frac{t_1^2 + \cdots + t_n^2}{2}}$.

Example 9. Consider the representation of $\mathbb{C}[x_1, \ldots, x_n]$ on $L^2(\mathbb{R})$, where $X_j s = t_j s$ for $s \in \mathcal{S}(\mathbb{R}^n)$. The unit vector $u = \pi^{-\frac{n}{4}} e^{-\frac{t_1^2 + \cdots + t_n^2}{2}}$ is cyclic for this representation. The faithful vector state is then given by

$$\phi(X_1^{d_1} \cdots X_n^{d_n}) = \begin{cases} \prod_{j=1}^n 2^{-\frac{d_j}{2}} (d_j - 1)!! & \text{if } d_1, \ldots, d_n \text{ are all even,} \\ 0 & \text{otherwise.} \end{cases}$$

Again, let us view ϕ as a functional on the $\star$-algebra $\mathbb{C}[x_1, \ldots, x_n]$, and let $f \in \mathbb{R}[x_1, \ldots, x_n]$. Observe that f is nonnegative on $\mathbb{R}^n$ if and only if $f(X_1, \ldots, X_n)$ is positive semidefinite. Also, note that $\phi(h^\star fh) = \phi((\frac{h+\bar{h}}{2})^2 f) + \phi((\frac{h-\bar{h}}{2i})^2 f)$ for $h \in \mathbb{C}[x_1, \ldots, x_n]$. Thus, $f \geq 0$ on $\mathbb{R}^n$ if and only if $\phi(h^2 f) \geq 0$ for all $h \in \mathbb{R}[x_1, \ldots, x_n]$ by Corollary 7.

3.3.1 A pushforward counterexample

In this subsection we give an example to show that Corollary 7 does not admit an analog of part (iv) in Theorem 3. The failure of the pushforward hierarchy in the unbounded case and its thorough analysis was first presented in [SW24]; our example gives an alternative shorter proof.

Consider the representation of $\mathbb{C}[x]$ on $L^2(\mathbb{R})$ given by $Xs = ts$, and its faithful vector state

$$\phi(a) = \int_{\mathbb{R}} a(t) \frac{e^{-t^2}}{\sqrt{\pi}} \, \mathrm{d}t$$

as in Example 9. Let $f = (x-1)^6 - \varepsilon$ for $\varepsilon > 0$. Since f is not a nonnegative polynomial, the unbounded operator $f(X)$ on $L^2(\mathbb{R})$ is not positive semidefinite; in particular, there exists $h \in \mathbb{R}[x]$ such that $\phi(h^2 f) < 0$.

On the other hand, we claim that if $\varepsilon > 0$ is small enough, then $\phi(p(f)^2 f) \geq 0$ for all univariate polynomials p. To see this, denote

$$\tilde{q} : \mathbb{R}_{\geq 0} \to \mathbb{R}, \quad \tilde{q}(y) = \left(\cos\left(2\sqrt{3}y^{\frac{1}{3}}\right) - \sqrt{3}\sin\left(2\sqrt{3}y^{\frac{1}{3}}\right)\right) e^{-y^{\frac{1}{3}}},$$

$$q : \mathbb{R} \to \mathbb{R}, \qquad q(t) = \tilde{q}\left((t-1)^6\right) e^{2(t-1)} = \left(\cos\left(2\sqrt{3}(t-1)^2\right) - \sqrt{3}\sin\left(2\sqrt{3}(t-1)^2\right)\right) e^{1-t^2}.$$

Observe that q is bounded on $\mathbb{R}$, and $q(1) = 1$. For $n \in \mathbb{N}_0$, let us calculate

$$m_n = \int_{\mathbb{R}} q(t)(t-1)^{6n} e^{-t^2} \, \mathrm{d}t$$

$$= \int_0^\infty \left(q(y^{\frac{1}{6}} + 1) e^{-2y^{\frac{1}{6}}} + q(-y^{\frac{1}{6}} + 1) e^{2y^{\frac{1}{6}}} \right) y^n e^{-y^{\frac{1}{3}} - 1} \frac{y^{-\frac{5}{6}}}{6} \, \mathrm{d}y$$

$$= \frac{1}{3e} \int_0^\infty \tilde{q}(y) y^{n-\frac{5}{6}} e^{-y^{\frac{1}{3}}} \, \mathrm{d}y,$$
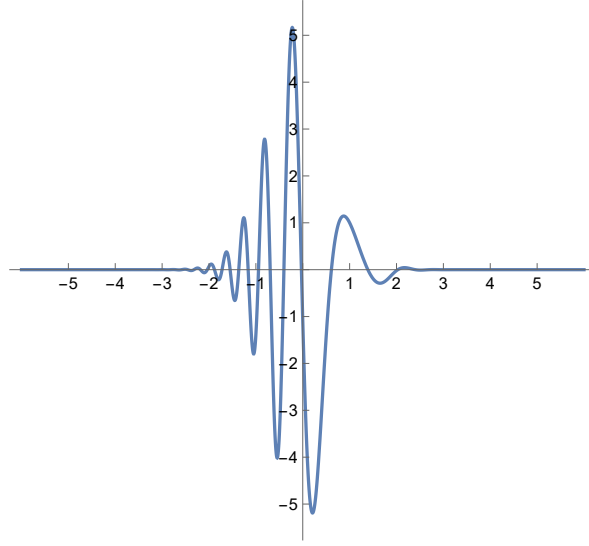
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Figure 1: Graph of the function q.

where we substituted $t - 1 = \pm\sqrt[6]{y}$. By [Ber88, Proposition 2],

$$\int_0^\infty \left(\cos\left(\sqrt{3}y^{\frac{1}{3}}\right) - \sqrt{3}\sin\left(\sqrt{3}y^{\frac{1}{3}}\right)\right) y^{n-\frac{5}{6}} e^{-y^{\frac{1}{3}}}\, \mathrm{d}y = 0$$

for all $n \in \mathbb{N}_0$ (using the integral representation of the gamma function). Consequently,

$$\int_0^\infty \tilde{q}(y) y^{n-\frac{5}{6}} e^{-y^{\frac{1}{3}}}\, \mathrm{d}y = \int_0^\infty \left(\cos\left(2\sqrt{3}y^{\frac{1}{3}}\right) - \sqrt{3}\sin\left(2\sqrt{3}y^{\frac{1}{3}}\right)\right) y^{n-\frac{5}{6}} e^{-2y^{\frac{1}{3}}}\, \mathrm{d}y$$

$$= 2^{\frac{5}{6}-n} \int_0^\infty \left(\cos\left(2\sqrt{3}y^{\frac{1}{3}}\right) - \sqrt{3}\sin\left(2\sqrt{3}y^{\frac{1}{3}}\right)\right) (2y)^{n-\frac{5}{6}} e^{-2y^{\frac{1}{3}}}\, \mathrm{d}y = 0,$$

and so $m_n = 0$ for all $n \in \mathbb{N}_0$. Since q is analytic, bounded and $q(1) > 0$, there exist $\eta, \varepsilon > 0$ such that $(t-1)^6 + \eta q(t) \geq \varepsilon$ for all $t \in \mathbb{R}$. Then for every univariate polynomial p,

$$\phi\left(p(f)^2 f\right) = \int_{\mathbb{R}} p\left((t-1)^6 - \varepsilon\right)^2 \left((t-1)^6 - \varepsilon\right) \frac{e^{-t^2}}{\sqrt{\pi}}\, \mathrm{d}t$$

$$= \int_{\mathbb{R}} p\left((t-1)^6 - \varepsilon\right)^2 \left((t-1)^6 - \varepsilon + \eta q(t)\right) \frac{e^{-t^2}}{\sqrt{\pi}}\, \mathrm{d}t \geq 0,$$

where we used the fact that $m_n = 0$ for all $n \in \mathbb{N}_0$.

3.4 Complete hierarchies of upper bounds

Let us consider a C^*-algebra $\mathcal{A}$ with a finite generating set S. As in [KMMV24, Section 3], we first recall the definition of localizing matrix. Given an order on S, let S_d be the list of $*$-words in S of length at most d, sorted with respect to the degree-lexicographic order. For every $d \in \mathbb{N}$ and $f = f^* \in \mathcal{A}$, the d-th order localizing matrix associated with a state ϕ on $\mathcal{A}$ and f is

$$\mathbf{M}_{S,d}(f\,\phi) := \left(\phi(u^* f v)\right)_{u,v \in S_d}.$$

When $S = \{f\}$, one simply writes

$$\mathbf{M}_{k,d}(f\,\phi) := \mathbf{M}_{\{f\},d}(f^k\,\phi) = \left(\phi(f^{i+j+k})\right)_{i,j=0}^d$$

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for all $k \geq 0$. Similarly to [KMMV24, Corollary 2], we derive a hierarchy of generalized eigenvalue problems converging to the minimum of the spectrum of f (i.e., its ground state energy), that is

$$\sigma_{\min}(f) = \sup\{\alpha \in \mathbb{R}: f - \alpha 1 \succeq 0\}.$$

Even though Corollary 10 is similar to [KMMV24, Corollary 2], the latter was based on the incorrect [KMMV24, Theorem 1] (see Remark 4), and erroneously made a general monotonicity assertion. We now provide a corrected statement and proof based on Theorem 3.

Corollary 10. *Let $\mathcal{A}$ be a C^*-algebra, S its generating set, and $(\phi_d)_{d=1}^{\infty}$ a sequence of states on $\mathcal{A}$ converging to a faithful state ϕ. For $f = f^* \in \mathcal{A}$ and $d \in \mathbb{N}$ denote*

$$\lambda_d = \max\left\{\lambda \in \mathbb{R}: \mathbf{M}_{S,d}(f\,\phi_d) \succeq \lambda \mathbf{M}_{S,d}(1\,\phi_d)\right\},$$
$$\eta_d = \max\left\{\eta \in \mathbb{R}: \mathbf{M}_{1,d}(f\,\phi_d) \succeq \eta \mathbf{M}_{0,d}(f\,\phi_d)\right\}.$$

Then the sequences $(\lambda_d)_d$ and $(\eta_d)_d$ are bounded by $\sigma_{\min}(f)$ from below, and

$$\lim_{d\to\infty} \lambda_d = \lim_{d\to\infty} \eta_d = \sigma_{\min}(f).$$

If furthermore $\phi_d = \phi$ for all $d \in \mathbb{N}$, then $(\lambda_d)_d$ and $(\eta_d)_d$ are nonincreasing sequences.

Proof. Let $\lambda = \sigma_{\min}(f)$. Then $f - \lambda \succeq 0$ in $\mathcal{A}$, so $\lambda_d, \eta_d \geq \lambda$ for all $d \in \mathbb{N}$ by Theorem 3. Now let $\varepsilon > 0$ be arbitrary, and let $\phi = \lim_d \phi_d$. Then $f - \lambda - \varepsilon \not\succeq 0$ in $\mathcal{A}$, so by Theorem 3 there exists $h \in \mathbb{C}\langle S\rangle$ such that $\phi(h^*(f - \lambda - \varepsilon)h) < 0$. Therefore, $\phi_d(h^*(f - \lambda - \varepsilon)h) < 0$ for all large enough $d \in \mathbb{N}$, so $\lambda_d < \lambda + \varepsilon$ for all large enough d. Hence, $\lim_d \lambda_d = \lambda$. Analogously we see that $\lim_d \eta_d = \lambda$.

Lastly, if $(\phi_d)_d$ is a constant sequence ϕ, then $\lambda_d \geq \lambda_{d+1}$ and $\eta_d \geq \eta_{d+1}$ because $\mathbf{M}_{S,d}(f\,\phi) - \lambda\mathbf{M}_{S,d}(1\,\phi)$ (resp. $\mathbf{M}_{1,d}(f\,\phi) - \eta\mathbf{M}_{0,d}(f\,\phi)$) is a submatrix of $\mathbf{M}_{S,d+1}(f\,\phi) - \lambda\mathbf{M}_{S,d+1}(1\,\phi)$ (resp. $\mathbf{M}_{1,d+1}(f\,\phi) - \eta\mathbf{M}_{0,d+1}(f\,\phi)$). ∎

The sequences $(\lambda_d)_d$ and $(\eta_d)_d$ are the noncommutative analogues of the sequences recalled in (2) and (4), of upper bounds for standard polynomial optimization from [Las11b] and [Las21], respectively. Each sequence element can be computed by solving a generalized eigenvalue problem.

Remark 11. To give a concrete example of a C^*-algebra that does not admit an efficiently computable separating sequence of states, consider $\mathcal{A} = \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m} \times \mathbb{Z}^{\star n}) \cong \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\max} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ for $m, n > 2$. By [MNY22, Figure 1], approximating $\sigma_{\min}(f)$ in $\mathcal{A}$ for every $f \in \mathbb{Z}^{\star m} \times \mathbb{Z}^{\star n}$ being computationally infeasible is equivalent to an equality of complexity classes $\mathtt{MIP}^{\mathtt{co}}{=}\mathtt{coRE}$, which has recently been established [Lin25] (see [AM25, Fact 3.2]). If $\mathcal{A}$ admitted a computable separating sequence of states, then one would have computable upper (Corollary 10) and lower ([HM04, PNA10]) bounds converging to $\sigma_{\min(f)}$ in $\mathcal{A}$, contradicting $\mathtt{MIP}^{\mathtt{co}}{=}\mathtt{coRE}$.

Finally, Corollary 7 yields the following weaker analog of Corollary 10 for unbounded operator algebras.

Corollary 12. *Let $\mathcal{O}$ be a closed O^*-algebra with domain $\mathcal{D}$, and ϕ a faithful vector state on $\mathcal{O}$. Suppose $\mathcal{O}$ is generated by a finite set S as a $*$-algebra. For $f = f^* \in \mathcal{O}$ and $d \in \mathbb{N}$ denote*

$$\lambda_d = \max\left\{\lambda \in \mathbb{R}: \mathbf{M}_{S,d}(f\,\phi) \succeq \lambda\mathbf{M}_{S,d}(1\,\phi)\right\}.$$

Then $(\lambda_d)_d$ is nonincreasing sequence, and

$$\lim_{d\to\infty} \lambda_d = \inf\{\langle fu, u\rangle: u \in \mathcal{D},\ \|u\| = 1\}.$$

For consistency with the C^*-algebra context, we denote $\sigma_{\min}(f) := \inf\{\langle fu, u\rangle: u \in \mathcal{D},\ \|u\| = 1\}$ (even though this infimum may not be a minimum, and equals $-\infty$ if f is unbounded from below).

Given a self-adjoint element f of a finitely generated C^*-algebra $\mathcal{A}$, Corollary 10 gives two sequences of generalized eigenvalue problems whose solutions converge to the spectral minimum of f, as long as there is an separating sequence of states on $\mathcal{A}$ that is efficiently computable (note that the converging sequence (5) is then likewise computable). Analogously, inner product (numerical range) optimization in an O^*-algebra is handled by Corollary 12.

4 Bell inequalities

We now apply the previously established framework to derive lower bounds on the maximal violation levels of Bell inequalities. A particularly notable example is the CHSH inequality introduced in [CHSH69], which considers a quantum system in which each party performs one of two possible measurements, each yielding outcomes in the set $\{\pm 1\}$. These measurements can be modeled by four self-adjoint unitary operators x_1, x_2, y_1, y_2 satisfying $x_i^2 = 1 = y_j^2$. To capture the non-local characteristics of the quantum system, we impose the additional requirement that the operators x_i act on one Hilbert space, while the operators y_j act on a distinct Hilbert space. The maximal violation of the CHSH inequality then corresponds to $-\sigma_{\min}(f)$, where

$$f = -x_1 \otimes y_1 - x_1 \otimes y_2 - x_2 \otimes y_1 + x_2 \otimes y_2,$$

which acts on the tensor product of the two Hilbert spaces, subject to the aforementioned unitary and locality (commutativity) constraints.

More generally, we consider a bipartite Bell scenario, where the parties have m and n inputs, respectively, and binary outputs. A Bell inequality for such a scenario is given by a (quadratic) polynomial f in self-adjoint unitaries[1] $x_1, \ldots, x_m$ and $y_1, \ldots y_n$, where the x_i's commute with the y_j's, such that f is positive semidefinite in the separable C^*-algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$. The analysis of positivity in this C^*-algebra depends on m and n, as follows.

Proposition 13. *Let $m, n \in \mathbb{N}$, and $G = \mathbb{Z}_2^{\star m} \times \mathbb{Z}_2^{\star n}$. The following holds.*

(a) *If $m, n \leq 2$, then $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n}) \cong \mathrm{C}^*_{\mathrm{red}}(G)$, and thus every $f = f^* \in \mathbb{C}[G]$ attains its spectral minimum in $\mathrm{C}^*_{\mathrm{red}}(G)$.*

(b) *If $m \geq 3$ or $n \geq 3$, the linear polynomial $(g_1 + \cdots + g_m) \otimes 1 + 1 \otimes (g_1 + \cdots + g_n) \in \mathbb{R}[G]$, where g_i denotes the generator of $\mathbb{Z}_2$ in the ith free factor, does not attain its spectral minimum in $\mathrm{C}^*_{\mathrm{red}}(G)$.*

Proof. The proof boils down to *amenability* of G. For a comprehensive study of amenable groups, see [Tak03, Chapter XIII] or [Jus22]. For our purposes, it suffices to apply known results on amenability, without going into an actual definition of amenability.

(a) Let $m, n \leq 2$. Note that G is finite if $m = n = 1$, has linear growth if only one of m, n equals 2, and quadratic growth if $m = n = 2$. Thus, G is amenable by [Tak03, Theorem XIII.4.7] or [Jus22, Section 2.6], and then (a) holds by [Tak03, Theorem XIII.4.6].

(b) Let $m \geq 3$ or $n \geq 3$. The group $\mathbb{Z}_2 \star \mathbb{Z}_2 \star \mathbb{Z}_2$ contains the free group on two generators as a subgroup (e.g., $g_1 g_3$ and $g_2 g_3$ are free). Thus, G contains the free group on two generators, in which case it is not amenable by [Tak03, Example XIII.4.4]. Hence, the spectral minimum of $(g_1 + \cdots + g_n) \otimes 1 + 1 \otimes (g_1 + \cdots + g_m)$ in $\mathrm{C}^*_{\mathrm{full}}(G)$ is strictly smaller than its spectral minimum in $\mathrm{C}^*_{\mathrm{red}}(G)$ by [Kes59a, §3 Theorem] as in Remark 6. ∎

Let $G = \mathbb{Z}_2^{\star m} \times \mathbb{Z}_2^{\star n}$. When minimizing $f = f^*$ in $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$, we thus distinguish two cases.

4.1 $m, n \leq 2$

In this case, the algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$ is isomorphic to $\mathrm{C}^*_{\mathrm{red}}(G)$ by Proposition 13. On $\mathrm{C}^*_{\mathrm{red}}(G)$, there is the canonical faithful state τ given by

$$\tau(\mathrm{id}) = 1, \qquad \tau(g) = 0 \quad \text{for } \mathrm{id} \neq g \in \mathbb{Z}_2^{\star m} \times \mathbb{Z}_2^{\star n}$$

---

[1] In Bell inequalities, the measurement operators are sometimes formulated as being projections; however, the affine coordinate change $x_i \mapsto 2x_i - 1$ maps projections to self-adjoint unitaries.

as in Example 5(1) above. Thus for $h \in \mathbb{C}[G]$, $\tau(h)$ is simply the constant term of h. For $d \in \mathbb{N}$ let $\mathbf{M}_d(h\,\tau)$ be the matrix indexed by words in G of length at most d, with the (u,v)-entry equal to $\tau(u^*hv)$. Note that $\mathbf{M}_d(1\,\tau) = \mathbf{I}_{s(d)}$, where $s(d)$ is the number of words $u,v \in G$ of length at most d. Given $f = f^* \in \mathbb{C}[G]$, we now consider the hierarchy of eigenvalue problems indexed by $d \in \mathbb{N}$:

$$
\begin{aligned}
\lambda_d = \max_{\lambda \in \mathbb{R}} \quad & \lambda \\
\text{s.t.} \quad & \mathbf{M}_d(f\,\tau) \succeq \lambda\,\mathbf{I}_{s(d)},
\end{aligned}
\tag{7}
$$

Corollary 10 implies that $(\lambda_d)_d$ converges monotonically to the minimum of f in $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$.

While the above illustrates an instance of an application of our results, we wish to point out that minimization of $f \in \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star 2}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star 2})$ can be also viewed as commutative polynomial optimization. Namely, $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star 2})$ embeds into 2×2 matrices over trigonometric polynomials; see (10) below. Then, $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star 2}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star 2})$ embeds into 4×4 matrices over bivariate trigonometric polynomials. Eigenvalue minimization of such matrices can be done using classical polynomial optimization tools.

4.2 General $m, n \in \mathbb{N}$

If $m \geq 3$ or $n \geq 3$, there exists $f = f^* \in \mathbb{C}[G]$ whose minimum $\sigma_{\min}(f)$ in $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$ is strictly lower than the limit of the hierarchy (7). Our strategy, initially given in [KMMV24, Section 3.2], to obtain upper bounds converging to $\sigma_{\min}(f)$ relies on tensor products of separating sequences (6) from Section 3.4 and a parameterization of self-adjoint unitaries by unitaries and signatures. That is, every self-adjoint unitary X of size d is of the form $X = U \begin{bmatrix} \mathbf{I}_r & 0 \\ 0 & -\mathbf{I}_{d-r} \end{bmatrix} U^*$ for some $r \leq d$ and $U \in \mathrm{U}_d(\mathbb{C})$. It turns out that it is sufficient to consider only X of even size $2d$ with $r = d$. One can then consider the (tracial) state that on a word w in $x_1, \ldots, x_n$ evaluates as

$$
\frac{1}{2d} \int_{U \in \mathrm{U}_{2d}(\mathbb{C})^n} \mathrm{tr}\left[w\left(U_1 \begin{bmatrix} \mathbf{I}_d & 0 \\ 0 & -\mathbf{I}_d \end{bmatrix} U_1^*, \ \ldots, U_n \begin{bmatrix} \mathbf{I}_d & 0 \\ 0 & -\mathbf{I}_d \end{bmatrix} U_n^* \right) \right] \mathrm{d}U.
$$

Such integrals with the respect to the Haar measure on unitary groups can be evaluated using the Weingarten calculus [CS06, CMN22]. Since $\mathrm{tr}(w_1 \otimes w_2) = \mathrm{tr}(w_1)\,\mathrm{tr}(w_2)$ for words w_1 in the x_i's and words w_2 in the y_j's, one relies on products of such state evaluations when preparing the generalized eigenvalue problems as in Corollary 10. We now formally justify the above strategy issued from [KMMV24, Section 3.2], by proving the following statement that narrows down the domain where $\sigma_{\min}(f)$ is attained.

Proposition 14. *Let $f = f^* \in \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$. We view f as a polynomial in $m + n$ self-adjoint unitary variables $x_1, \ldots, x_m, y_1, \ldots, y_n$. Then*

$$
\begin{aligned}
\sigma_{\min}(f) = \inf_{d,e \in \mathbb{N}} \min\Big\{ &\, \mathrm{mineig}\, f(X_1 \otimes I_e, \ldots, X_m \otimes I_e, I_d \otimes Y_1, \ldots, I_d \otimes Y_n) : \\
&\, X_i = X_i^* \in \mathrm{U}_d(\mathbb{C}), Y_j = Y_j^* \in \mathrm{U}_e(\mathbb{C}) \Big\} \\
= \inf_{d \in \mathbb{N}} \min\Big\{ &\, \mathrm{mineig}\, f(X_1 \otimes I_d, \ldots, X_m \otimes I_d, I_d \otimes Y_1, \ldots, I_d \otimes Y_n) : \\
&\, X_i = X_i^*, Y_j = Y_j^* \in \mathrm{U}_{2d}(\mathbb{C}), \mathrm{tr}\, X_i = \mathrm{tr}\, Y_j = 0 \Big\}.
\end{aligned}
\tag{8}
$$

Proof. The first equality in (8) holds because $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$ is a residually finite-dimensional algebra (see for instance [KVV17, Proposition A.2]), and then so is $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$ by the definition of the spatial tensor product $\otimes_{\min}$. The $\leq$ part of the second equality in (8) is clear. Conversely, let $X_i = X_i^* \in \mathrm{U}_d(\mathbb{C}), Y_j = Y_j^* \in \mathrm{U}_e(\mathbb{C})$ be arbitrary, and let $k \geq d + \max_i |\mathrm{tr}\, X_i|, e + \max_j |\mathrm{tr}\, Y_j|$ be

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an even number. Then one can find diagonal matrices $D_i \in \mathrm{M}_{k-d}(\mathbb{C}), E_j \in \mathrm{M}_{e-d}(\mathbb{C})$ with ± 1 on the diagonal such that the $k \times k$ self-adjoint unitaries $X_i' = X_i \oplus D_i, Y_j' = Y_j \oplus E_j$ satisfy $\mathrm{tr}\, X_i' = \mathrm{tr}\, Y_j' = 0$. Clearly,

$$\mathrm{mineig}\, f(X_i \otimes I, I \otimes Y_j) \geq \mathrm{mineig}\, f(X_i' \otimes I, I \otimes Y_j')$$

holds. Since X_i, Y_j were arbitrary, the $\geq$ part of the second equality in (8) follows. ∎

Note that every $X = X^* \in \mathrm{U}_{2d}(\mathbb{C})$ with $\mathrm{tr}\, X = 0$ is unitarily equivalent to $S = \left(\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix} \right)$ with $d \times d$ blocks. In analogy with Example 5(e), Proposition 14 implies that

$$\psi_d(u \otimes v) = \frac{1}{4d^2} \left(\int_{U \in \mathrm{U}_{2d}(\mathbb{C})^m} \mathrm{tr}\, u(U_1 S U_1^*, \ldots, U_n S U_n^*)\, \mathrm{d}U \right)$$
$$\cdot \left(\int_{V \in \mathrm{U}_{2d}(\mathbb{C})^n} \mathrm{tr}\, v(V_1 S V_1^*, \ldots, V_m S V_m^*)\, \mathrm{d}V \right) \tag{9}$$

is a separating sequence of states for $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\mathrm{min}} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$, computable via the Weingarten calculus. By Corollary 10, this separating sequence gives rise to a hierarchy of generalized eigenvalue problems whose solutions converge to $\sigma_{\mathrm{min}}(f)$.

5 Numerical examples

Our experiments were performed on an Apple Macbook Air M2 with 16GB of RAM in Wolfram Mathematica 14.2.

5.1 Bell inequalities

Example 15. We consider the tilted CHSH inequality [AMP12], where

$$f_\alpha = \alpha x_1 + x_1 y_1 + x_1 y_2 + x_2 y_1 - x_2 y_2,$$

$\alpha \in [0, 2)$ is a parameter, and the four self-adjoint operators x_1, x_2, y_1, y_2 satisfy $x_i^2 = 1 = y_j^2$ and $x_i y_j = y_j x_i$. The largest violation of f, i.e., $\sigma_{\mathrm{max}}(f_\alpha) = -\sigma_{\mathrm{min}}(-f_\alpha)$, is known to be $\sqrt{8 + 2\alpha^2}$. In the case $\alpha = 0$, f_α reduces to the function involved in the CHSH inequality, already discussed at the beginning of Section 4.

With the canonical faithful state τ defined in Section 4.1 and the hierarchy from (7), we report on Figures 2–4 (resp. Figure 5) the values of λ_d for $d \leq 100$ (resp. 50) and a few selected values of α. The dashed line represents the analytical value of the minimum, i.e., $\lim_{d \to \infty} \lambda_d$. The corresponding computation time is less than an hour. The first displayed dotted curve fits with the function $d \mapsto \sigma_{\mathrm{min}}(-f_{1/4}) + 5d^{-1.75}$, so for this particular example we conjecture a heuristic estimate of $O(d^{-1.75})$ for the convergence rate. We conjecture similar super-linear estimates of $O(d^{-1.63})$, $O(d^{-1.65})$ for the second and three cases, and a super-quadratic estimate of $O(d^{-2.23})$ for the last one.

For the usual CHSH inequality, we also refer to the numerical results from [KMMV24, Section 3.2] for preliminary experiments based on the separating state sequence from Section 4.2, given in (9).

5.2 Weyl algebras

Example 16. Here we illustrate our approximation framework in the unbounded operator setting, for the Weyl algebra $\mathcal{W} = \mathbb{C}\langle x, y \colon xy - yx = 1 \rangle$ with $x^\star = -x$ and $y^\star = y$, previously mentioned in Example 8. After the linear change of variables $a = \frac{x+y}{\sqrt{2}}, a^\star = \frac{y-x}{\sqrt{2}}$, one has $\mathcal{W} = \mathbb{C}\langle a, a^\star \colon aa^\star - a^\star a = 1 \rangle$. The
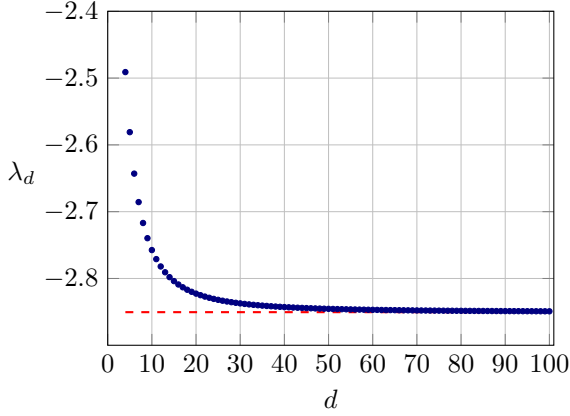
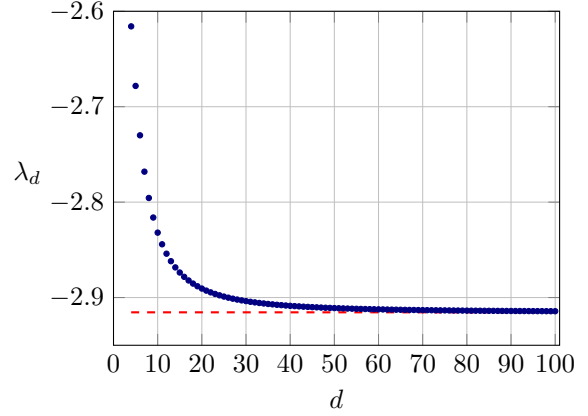Figure 2: λ_d for $d \leq 100$ in Example 15 for $\alpha = \frac{1}{4}$.   Figure 3: λ_d for $d \leq 100$ in Example 15 for $\alpha = \frac{1}{2}$.
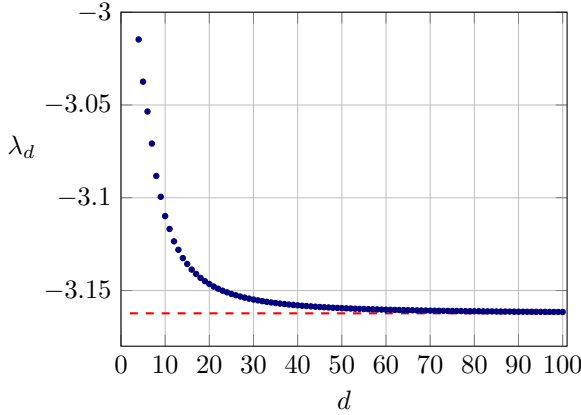

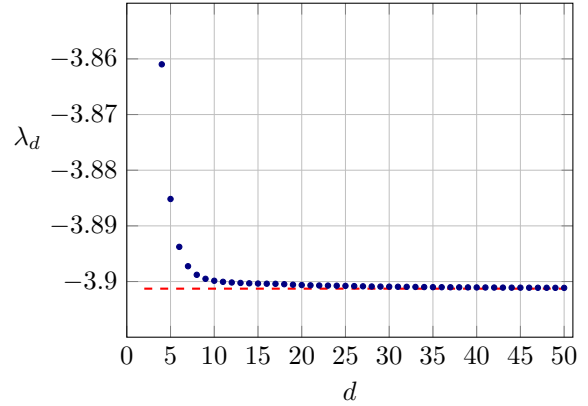Figure 4: λ_d for $d \leq 100$ in Example 15 for $\alpha = 1$.   Figure 5: λ_d for $d \leq 50$ in Example 15 for $\alpha = 1.9$.

commutation relation implies that every element in $\mathcal{W}$ is of the form $\sum_{m,n=0}^{d} \gamma_{mn} a^{\star m} a^n$ for $\gamma_{mn} \in \mathbb{C}$ (i.e., it looks like a "commutative" polynomial). Consider the faithful vector state ϕ given by

$$\phi(a^{\star m} a^n) = \begin{cases} 1 & \text{if } m = n = 0, \\ 0 & \text{otherwise.} \end{cases}$$

For $h \in \mathcal{W}$ let $\mathbf{M}_d(h\,\phi)$ be the $(d+1)^2 \times (d+1)^2$ matrix indexed by $a^{\star m} a^n$ for $m, n \leq d$, whose $(a^{\star k} a^\ell, a^{\star m} a^n)$-entry equals $\phi(a^{\star \ell} a^k h\, a^{\star n} a^m)$. Given $f \in \mathcal{W}$, Example 8 and Corollary 12 show that the values

$$\lambda_d = \max \left\{ \lambda \in \mathbb{R} \colon \mathbf{M}_d(f\,\phi) \succeq \lambda \mathbf{M}_d(1\,\phi) \right\}$$

form a decreasing sequence converging to $\sigma_{\min}(f)$.

We consider several examples from [Cim10] where the author derives a hierarchy of lower bounds computable by semidefinite programming, and based on representations of positive polynomials in Weyl algebras by Schmüdgen [Sch05].

(a) We start with the polynomial $f_1 = (x^2 - y^2)^2$ from [Cim10, Example 1]. The first order of the lower bound hierarchy from [Cim10] provides the value $1 \leq \sigma_{\min}(f_1)$. After applying the change of

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variable $a = \frac{x+y}{\sqrt{2}}$, one has $f_1 = 1 + 8a^\star a + 4a^{\star 2}a^2$, thus $\phi(f_1) = \lambda_0(f_1) = 1$. This proves that 1 is an upper bound for $\sigma_{\min}(f_1)$, implying that $\sigma_{\min}(f_1) = 1$.

(b) Next we consider $f_2 = -x^2 + y^2 + \beta y^4$ as in [Cim10, Example 2]. Accurate approximation of $\sigma_{\min}(f_2)$ for various β are reported in [Ban78, Table 1].

Results for $\beta = 1$ are reported (up to 6 digits) in Table 1. They were computed symbolically in Mathematica by solving a generalized eigenvalue problem. The value from [Ban78] is $\sigma_{\min}(f_2) \simeq$

d	1	2	3	4	5	6
λ_d	1.750000	1.412603	1.412603	1.395071	1.395071	1.394907

Table 1: Computational results for $\beta = 1$.

1.392352.

For $\beta = 0.1$ the results are given in Table 2. The value from [Ban78] is $\sigma_{\min}(f_2) \simeq 1.065286$.

d	1	2	3	4	5	6
λ_d	1.075000	1.065833	1.065833	1.065376	1.065376	1.065287

Table 2: Computational results for $\beta = 0.1$.

(c) Finally, we consider the polynomial $f_3 = x^4 + y^4$ from [Cim10, Example 1]. The second order of the lower bound hierarchy from [Cim10] yields the value $1.396726 \leq \sigma_{\min}(f_3)$. The values provided by our complementary upper bound hierarchy are given in Table 3.

d	1	2	3	4	5	6	7	8
λ_d	3/2	3/2	3/2	1.400166	1.400166	1.400166	1.400166	1.396835

Table 3: Computational results for f_3.

5.3 Motzkin polynomial

Example 17. Consider the Motzkin polynomial $f = 1 - 3x^2y^2 + x^4y^2 + x^2y^4 \in \mathbb{R}[x, y]$. It is well known that f is a nonnegative polynomial, with minimum 0 attained on $\{-1, 1\}^2$, and $f + \lambda$ is not a sum of squares in $\mathbb{R}[x, y]$ for any $\lambda \in \mathbb{R}$. Let $\phi : \mathbb{R}[x, y] \to \mathbb{R}$ be the linear functional given as

$$\phi(x^m y^n) = \begin{cases} 2^{-\frac{m+n}{2}}(m-1)!!(n-1)!! & \text{if both } m \text{ and } n \text{ are even} \\ 0 & \text{otherwise.} \end{cases}$$

For $h \in \mathbb{R}[x, y]$ let $\mathbf{M}_d(h\,\phi)$ be the $\binom{d+2}{2} \times \binom{d+2}{2}$ matrix indexed by $x^m y^n$ for $m + n \leq d$, whose $(x^k y^\ell, x^m y^n)$-entry equals $\phi(x^{k+m} y^{\ell+n} h)$. Example 9 and Corollary 12 (also [Las11b, Example 1] for a different choice of the functional), show that the values

$$\lambda_d = \max\left\{\lambda \in \mathbb{R} : \mathbf{M}_d(f\,\phi) \succeq \lambda \mathbf{M}_d(1\,\phi)\right\}$$

form a nonincreasing sequence converging to $\min_{\mathbb{R}^2} f$. For example,

$$\lambda_1 = 1, \quad \lambda_2 = \lambda_3 = \frac{13 - 3\sqrt{10}}{4},$$

and Figure 6 lists the values of λ_d for $d = 1, \ldots, 34$. Here again, the figure confirms that the sequence gets reasonably close to the minimum of f when d increases. The displayed dotted curve fits with

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the function $d \mapsto \sigma_{\min}(f) + 3d^{-0.65}$, so for this particular example we conjecture a sublinear heuristic estimate of $O(d^{-0.65})$ for the convergence rate.
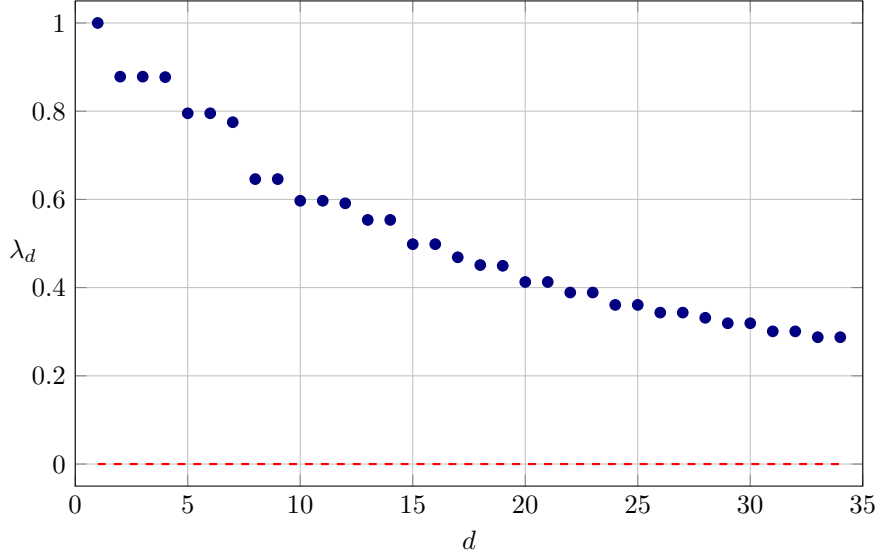

Figure 6: Values λ_d for $d \leq 34$ in Example 17

5.4 Optimizing an exponential function

Example 18. As in [AGN24, § V-B], consider the spectral minimum of $\exp(X_0 X_1 + X_1 X_0)$ for arbitrary orthogonal projections X_0, X_1 on a Hilbert space.

The universal C^*-algebra

$$\mathcal{A} = \mathrm{C}^*\langle x_0, x_1 \colon x_j^2 = x_j^* = x_j \rangle$$

is isomorphic to $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2 \star \mathbb{Z}_2) = \mathrm{C}^*_{\mathrm{red}}(\mathbb{Z}_2 \star \mathbb{Z}_2)$ (via $x_j \mapsto 2x_j - 1 =: e_j$), and thus admits the canonical tracial state τ as in Example 5(a). We will apply Corollary 10 to τ and $f = e^{x_0 x_1 + x_1 x_0} \in \mathcal{A}$; first, we find an explicit formula for τ.

Let W denote the set of alternating words in x_0, x_1. Then the state τ depends only on the length of a word in W, so we let t_n denote the value of τ on a word of length n. By the cyclic property, $t_{2n+1} = t_{2n}$ for all positive integers n. Note that $t_0 = 1 \neq \frac{1}{2} = t_1$. To find the values of t_n, consider the representation of $\mathcal{A}$ within 2×2 matrices over continuous functions on the interval $[0, 2\pi]$,

$$
\begin{aligned}
\pi : \mathcal{A} &\to M_2(\mathcal{C}[0, 2\pi]), \\
x_0 &\mapsto \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \\
x_1 &\mapsto \frac{1}{2} \begin{bmatrix} 1 + \cos(\phi) & \sin(\phi) \\ \sin(\phi) & 1 - \cos(\phi) \end{bmatrix}.
\end{aligned}
\tag{10}
$$

Define the state

$$
\begin{aligned}
\tau' : \mathcal{A} &\to \mathbb{C}, \\
W \ni w &\mapsto \frac{1}{2\pi} \int_0^{2\pi} \mathrm{Tr}(\pi(w)) \, \mathrm{d}\phi,
\end{aligned}
$$

where Tr denotes the *normalized* trace on $M_2(\mathbb{C})$. We claim that $\tau' = \tau$. Observe that the group

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generators $e_j = 2x_j - 1$ of $\mathcal{A}$ are mapped under π into

$$\pi(e_0) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad \pi(e_1) = \begin{bmatrix} \cos(\phi) & \sin(\phi) \\ \sin(\phi) & -\cos(\phi) \end{bmatrix}.$$

Then for $r \in \mathbb{N}$,

$$\pi\big((e_0 e_1)^r\big) = \begin{bmatrix} \cos(r\phi) & \sin(r\phi) \\ -\sin(r\phi) & \cos(r\phi) \end{bmatrix},$$

whence

$$\tau'\big((e_0 e_1)^r\big) = \frac{1}{2\pi} \int_0^{2\pi} \cos(r\phi)\, d\phi = \begin{cases} 1 & r = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, $\tau'\big((e_0 e_1)^r e_0\big) = 0$ for all r. By the (obvious) tracial property of τ' we deduce $\tau = \tau'$.

This makes it possible to evaluate τ in terms of x_0, x_1. Namely,

$$\pi\big((x_0 x_1)^r\big) = \begin{bmatrix} \frac{1}{2^r}(1 + \cos(\phi))^r & * \\ 0 & 0 \end{bmatrix},$$

so

$$t_{2r} = \tau\big((x_0 x_1)^r\big) = \tau'\big((x_0 x_1)^r\big) = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{2^r}(1 + \cos(\phi))^r\, d\phi = \frac{\Gamma\left(r + \frac{1}{2}\right)}{2\sqrt{\pi}\,\Gamma(r+1)} = \frac{\Gamma\left(r + \frac{1}{2}\right)}{2\sqrt{\pi}\,r!}.$$

Let $f = e^{x_0 x_1 + x_1 x_0}$. Then

$$\pi(f) = \frac{1}{2} e^{-2\sin^2\left(\frac{\phi}{4}\right)\cos\left(\frac{\phi}{2}\right)}$$
$$\cdot \begin{bmatrix} \left(e^{2\cos\left(\frac{\phi}{2}\right)} - 1\right)\cos\left(\frac{\phi}{2}\right) + e^{2\cos\left(\frac{\phi}{2}\right)} + 1 & \sin\left(\frac{\phi}{2}\right)\left(e^{2\cos\left(\frac{\phi}{2}\right)} - 1\right) \\ \sin\left(\frac{\phi}{2}\right)\left(e^{2\cos\left(\frac{\phi}{2}\right)} - 1\right) & -\left(\left(e^{2\cos\left(\frac{\phi}{2}\right)} - 1\right)\cos\left(\frac{\phi}{2}\right)\right) + e^{2\cos\left(\frac{\phi}{2}\right)} + 1 \end{bmatrix},$$

and

$$\text{Tr}\left(\pi(f)\right) = \frac{1}{2} e^{-\cos\left(\frac{\phi}{2}\right) + \frac{\cos(\phi)}{2} + \frac{1}{2}} + \frac{1}{2} e^{\cos\left(\frac{\phi}{2}\right) + \frac{\cos(\phi)}{2} + \frac{1}{2}},$$

so

$$\tau(f) = \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{1}{2} e^{-\cos\left(\frac{\phi}{2}\right) + \frac{\cos(\phi)}{2} + \frac{1}{2}} + \frac{1}{2} e^{\cos\left(\frac{\phi}{2}\right) + \frac{\cos(\phi)}{2} + \frac{1}{2}} \right) d\phi.$$

However, $\tau(f)$ does not seem to have a closed-form expression, but is easy to compute numerically to desired precision ($\tau(f) \approx 2.33563$), so we proceed numerically.

We can now construct

$$\mathbf{M}_d(f\,\tau) = \left(\tau(u^* f v)\right)_{u,v \in W,\, |u|,|v| \le d}, \qquad \mathbf{M}_d(1\,\tau) = \left(\tau(u^* v)\right)_{u,v \in W,\, |u|,|v| \le d}$$

for $d \in \mathbb{N}$. By Corollary 10,

$$\lambda_d = \max\left\{\lambda \in \mathbb{R} \colon \mathbf{M}_d(f\,\tau) \succeq \lambda \mathbf{M}_d(1\,\tau)\right\}$$

is a decreasing sequence whose limit is the spectral minimum of $\exp(X_0 X_1 + X_1 X_0)$ for orthogonal projections X_0, X_1.

Figure 18 lists the values of λ_d for $d = 1, \ldots, 22$. Here again, the figure confirms that the sequence gets reasonably close to the minimum of f when d increases. The displayed dotted curve fits with the function $d \mapsto \sigma_{\min}(f) + 0.4 d^{-1.58}$, so for this particular example we conjecture a super-linear heuristic estimate of $O(d^{-1.58})$ for the convergence rate. The minimum in this example is $\sigma_{\min}(f) = \exp(-\frac{1}{4}) \approx 0.778801$.
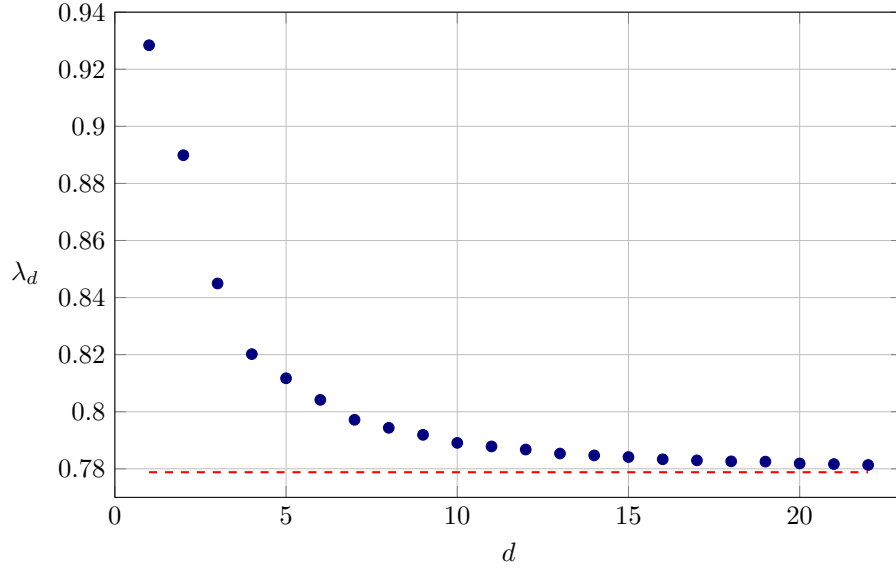
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Figure 7: Values λ_d for $d \leq 22$ in Example 18

6 Conclusion

We derived complete hierarchies of upper bounds for the spectral minimum of noncommutative polynomials. These are the noncommutative analogues of the Lasserre hierarchies approximating the minimum of commutative polynomials from above. As in the commutative case, each upper bound is computed through solving a generalized eigenvalue problem. We applied the derived hierarchies to both bounded and unbounded operator algebras, as well as non-polynomial analytic functions in noncommuting variables, demonstrating their flexibility and broad applicability.

In the commutative setting, despite the absence of empirical evidence indicating that the Lasserre hierarchy of upper bounds surpasses classical numerical approaches—such as brute-force sampling methods grounded in Monte Carlo techniques or local optimization algorithms employing gradient descent—the asymptotic properties of the upper bound hierarchy have been more thoroughly characterized than those of the lower bound hierarchy. In [dKLS16], the authors establish convergence rates that frequently align with empirical observations and are bounded above by $(O(1/\sqrt{d})$, where d denotes the relaxation order within the hierarchy. For certain specific domains, this convergence rate has been refined to $O(1/d^2)$, notably for the hypercube $[-1,1]^n$ as demonstrated in [DKHL17] and for the sphere as shown in [dKL22]. More recently, analogous convergence rates have been achieved for the standard hierarchy of lower bounds by [Slo22] through a synthesis of upper bound rates and a sophisticated application of Christoffel-Darboux kernels; for a comprehensive overview of these kernels, see the recent survey by [LPP22]. For the presented examples of this paper, we provided heuristic estimates for the convergence rate. A comprehensive and rigorous analysis of the convergence rate is beyond reach for the current framework, and is left to be explored in future studies.

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