Complete Upper Bound Hierarchies for Spectral Minimum in Noncommutative Polynomial Optimization

Igor Klep* Victor Magron† Jurij Volčič‡

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Abstract

This work focuses on finding the spectral minimum (ground state energy) of a noncommutative polynomial subject to a finite number of noncommutative polynomial constraints. Based on the Helton-McCullough Positivstellensatz, the Navascués-Pironio-Acín (NPA) hierarchy is the noncommutative analog of Lasserre's moment-sum of squares hierarchy and provides a sequence of *lower* bounds converging to the spectral minimum, under mild assumptions on the constraint set. Each lower bound can be obtained by solving a semidefinite program.

This paper derives complementary complete hierarchies of *upper* bounds for the spectral minimum. They are noncommutative analogues of the upper bound hierarchies due to Lasserre for minimizing commutative polynomials over compact sets. Each upper bound is obtained by solving a generalized eigenvalue problem. The derived hierarchies apply to optimization problems in bounded and unbounded operator algebras, as demonstrated on a variety of examples.

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*igor.klep@fmf.uni-lj.si Department of Mathematics, University of Ljubljana & Famnit, University of Primorska, Koper & Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

†vmagron@laas.fr LAAS-CNRS & Institute of Mathematics from Toulouse, France

‡jurij.volcic@auckland.ac.nz Department of Mathematics, University of Auckland, New Zealand

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 in several operator variables naturally arise in quantum physics; for example, Bell inequalities, initially introduced by [Bel64], that can be viewed as specific types of inequalities on eigenvalues of noncommutative polynomials; see [PNA10]. In the commutative setting, *polynomial optimization* aims at finding the minimum of a polynomial objective function under finitely many polynomial inequality constraints. As shown, e.g., in [Lau09], this optimization problem is NP-hard to solve exactly, thus a plethora of approximation schemes have been developed in the last two decades, in particular *the moment-sum of squares* (moment-SOS) hierarchy by [Las01], also known as the Lasserre hierarchy, that relies on the Positivstellensatz by [Put93]. At a given step of this hierarchy, the corresponding lower bound is computed by solving a semidefinite program, i.e., by minimizing a linear objective function under linear matrix inequality constraints; see [VB96]. The Lasserre hierarchy of lower bounds is ensured to converge to the polynomial minimum under mild natural assumptions often satisfied in practice, e.g., in the presence of a ball constraint. Similarly, minimal eigenvalues of noncommutative polynomials can be approximated by a lower bound hierarchy, also known as the Navascués-Pironio-Acín (NPA) hierarchy; see [DLTW08, NPA08, BKP16], that relies on the Positivstellensatz by Helton-McCullough [HM04]. Exactness of this approximation scheme is ensured under the same assumption as in the commutative case.

Back in the commutative setting, another hierarchy proposed in [Las11b] yields a monotone sequence of *upper bounds* which converges to the minimum of a polynomial on a given set, and therefore can be seen as complementary to the standard Lasserre hierarchy of lower bounds. At a given step of this hierarchy, the corresponding upper bound is computed by solving a so-called *generalized eigenvalue* problem. As for the lower bound hierarchy, the sizes of the involved matrix optimization variables are critical and restrict its use to small size problems. For the lower bound hierarchy, a common workaround consists of exploiting the structure, e.g., sparsity or symmetry of the input polynomials; see [MW23] for a recent survey on sparsity-exploiting techniques and [HKP24] for even more sophisticated structure exploitation techniques applied to Bell inequalities. A first attempt to improve practical efficiency of the upper bound hierarchy for polynomial optimization has been done in [Las21]. The idea is to use the pushforward measure of the uniform measure by the polynomial to be minimized. In doing so one reduces the initial problem to a related univariate problem and as a result one obtains another hierarchy of upper bounds which involves univariate sums of squares polynomials of increasing degree. When minimizing a given polynomial on a non-compact set, it was recently proved in [SW24] that this hierarchy may fail to converge to the global minimum.

By contrast with the commutative setting, obtaining upper bounds for minimal eigenvalues of noncommutative polynomials has been less explored. Existing methods include the density matrix renormalization group, e.g., by [Whi92], which is a numerical variational technique devised to obtain the low-energy physics of quantum many-body systems, or quantum variants of Monte-Carlo methods, e.g., by [NU98]. A first attempt has been done by [Ric20] to compute minimal eigenvalues of pure quartic oscillators, but without any convergence guarantees and lack of scalability.

Contributions

The goal of this work is to propose a comprehensive scheme for computing upper bounds in noncommutative minimization. We derive two complete upper bound hierarchies for spectral minima of noncommutative polynomials in C^*-algebras $\mathcal{A}$, and their analogs in O^*-algebras of unbounded operators. These hierarchies can be seen as the noncommutative analogues of [Las11b] and [Las21]. Similarly to the commutative case, the hierarchies are parametrized by the choice of either a faithful state on $\mathcal{A}$, or more generally, a *separating sequence* of states on $\mathcal{A}$, and a dense (formal) subalgebra of $\mathcal{A}$. In both cases, each upper bound is obtained by solving a single finite-dimensional generalized eigenvalue problem. The effectiveness of this approach relies on computability of states. While every separable C^*-algebra $\mathcal{A}$ admits faithful states, they do not always admit a closed form suitable for evaluation. However, often there are separating sequences of states that are effectively computable on a dense subalgebra of $\mathcal{A}$; one of the advantages of the derived hierarchies is their applicability to such separating state sequences. Our approach carries potential applications for estimating spectral minima of polynomial operators pertaining to partial differential equations, ground state energies of composite Hamiltonians in mathematical physics, and violations of probabilistic inequalities in quantum information theory. For example, our framework directly applies to approximate violations of Bell inequalities by considering tensor products of universal group C^*-algebras with separating state sequences, that can be evaluated using the calculus for Haar integration over unitary groups [CS06]. Furthermore, we test the presented hierarchies on polynomial differential operators in the Weyl algebra with the faithful vector state induced by the normal multivariate Gaussian, and non-polynomial analytic functions in noncommuting operator variables. For the presented examples, we also provide heuristic estimates for the convergence rate. A short preliminary version of this paper has been previously presented at the MTNS conference [KMMV24].

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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

$$\begin{aligned} L_{\mathbf{z}} :\ & \mathbb{R}[x] \to \mathbb{R} \\ f \left(= \sum_{\alpha\in\mathbb{N}^n} f_\alpha x^\alpha \right) & \mapsto L_{\mathbf{z}}(f) = \sum_{\alpha\in\mathbb{N}^n} f_\alpha z_\alpha. \end{aligned} \tag{1}$$

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, 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 $\mathbf{\Omega}$, let $f : \mathbf{X} \to \mathbf{\Omega} \subseteq \mathbb{R}$ be a polynomial 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 $C \in \mathcal{B}(\Omega)$, where $\mathcal{B}(\mathbf{\Omega})$ denotes the Borel algebra of $\mathbf{\Omega}$, 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

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

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

Let F be a noncommutative polynomial in m variables. We are interested in optimizing or deciding positive semidefiniteness of $F(X_1, \dots, X_m)$ over all tuples of operators $(X_1, \dots, X_m)$ satisfying given polynomial relations. Such operators can be often seen as representations of a single (typically very large) operator algebra $\mathcal{A}$, and the positivity of F on such operators is then equivalent to positivity of a single element $f \in \mathcal{A}$. For example, consider the problem of whether $F(U_1, \dots, U_n)$ is positive semidefinite for all tuples of unitaries $U_1, \dots, U_n$ acting on a separable Hilbert space. This is equivalent to $f = F(W_1, \dots, W_n)$ being positive semidefinite, where $W_1, \dots, W_n$ are the unitary generators of the universal group C^*-algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. Thus we develop our approach to noncommutative positivity eigenvalue optimization in terms of positivity of elements in operator algebras. Our goal is to approximate from above the minimum of the spectrum of f, i.e., $\sigma_{\min}(f) = \sup\{\alpha \in \mathbb{R} \colon f - \alpha 1 \succeq 0\}$. Note that the spectral minimum or 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, and $\sigma_{\min}(f) = 0$).

3.1 Positivity in C^*-algebras via faithful functionals

Let $\mathcal{A}$ be a (unital) C^*-algebra. Let us introduce some terminology pertaining to states (unital positive linear functionals) on $\mathcal{A}$ and $*$-subalgebras of $\mathcal{A}$ that is used in this section. A state ϕ on $\mathcal{A}$ is *faithful* if $\phi(a^*a) = 0$ implies $a = 0$ for $a \in \mathcal{A}$. A sequence of states $(\phi_d)_d$ on $\mathcal{A}$ is *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

$$\tilde{\phi}_d = \left(\frac{2^d}{2^d - 1} \sum_{i=1}^{d} \frac{1}{2^i} \phi_i \right)_{d=1}^{\infty}, \tag{5}$$

then $(\tilde{\phi}_d)_d$ converges (in the weak-* topology) to a faithful state on $\mathcal{A}$. Note that separable C^*-algebras (in particular, finitely generated C^*-algebras) always admit faithful states [Tak02, Exercise I.9.3, or proof of Theorem I.9.23]. Given a subset $S \subset \mathcal{A}$ let $\mathbb{C}\langle S \rangle_d$ denote the span of all $*$-words in S (i.e., products of elements of S and their adjoints) of length at most d, and let $\mathbb{C}\langle S \rangle$ denote the $*$-algebra generated by S. We say that S is *generating* if $\mathcal{A}$ is the closure in the strong operator topology of $\mathbb{C}\langle S \rangle$.

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 $f = f^* \in \mathbb{C}\langle S \rangle$, 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)⇒(ii)-(v) are clear.

(ii)⇒(i): Since S is generating, 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]. 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)⇒(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 $d \geq d_0$. Consequently, $\phi(h^* f h) \geq 0$.

(v)⇒(iv): The argument is analogous to (iii)⇒(ii).

(iv)⇒(i): Let $\mathcal{B}$ be the abelian C^*-subalgebra in $\mathcal{A}$ generated by f. By the proof (ii)⇒(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 $\mathcal{A}$. ∎

Example 4. The following are some well-known separable C^*-algebras and their faithful states, or separating sequences of states (which give rise to sequences converging to faithful states as in (5).

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

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

is faithful.

(b) The graph C^*-algebra of a finite graph Γ (in particular, the Cuntz algebra) 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

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

The separating property of (6) follows by [Cho80, Theorem 7] (cf. [KVV17, Corollary 4.7]). 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 $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. The states (6) can be efficiently evaluated using the Collins-Śniady calculus for Haar integration over unitary groups [CS06, Corollary 2.4].

(d) Suppose $\mathcal{A}_1$ and $\mathcal{A}_2$ are C^*-algebras with faithful states ϕ_1 and ϕ_2, respectively. Then the state $\phi_1 \otimes \phi_2$ on the minimal (injective) tensor product $\mathcal{A}_1 \otimes_{\min} \mathcal{A}_2$ is faithful [Tak02, Theorem IV.4.9], and the state $\phi_1 \star \phi_2$ on the reduced free product $\mathcal{A}_1 \star \mathcal{A}_2$ is faithful [Dyk98, Theorem 1.1]. Values of $\phi_1 \otimes \phi_2$ and $\phi_1 \star \phi_2$ are easily expressible with values of ϕ_1 and ϕ_2.

(e) Combining (c) and (d), one obtains an explicit separating sequence for the algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$. See Section 4 for more details. As a side remark, note that $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ is not isomorphic to $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\max} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n}) \cong \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m} \times \mathbb{Z}^{\star n})$ for $m, n \geq 2$ by 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 the positivity perspective.

Remark 5. Let G be the free group on n generators $S = \{g_1, \dots, g_n\}$. 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 $f(1,\dots,1) = \frac{\sqrt{2n-1}}{n} - 1 < 0$.

More generally, let G be a discrete group generated by n generators $g_1,\dots,g_n$, 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].

3.2 Positivity in O^*-algebras

Let us record an observation for unbounded operator algebras in the spirit of Theorem 3. 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 $\{v \mapsto \|av\| : a \in \mathcal{O}\}$). 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 $v \in \mathcal{O} \cdot u$. This leads to the following observation.

Proposition 6. *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 $h \in \mathcal{O}$.*

Proposition 6 is weaker than Theorem 3 in several aspects. While Theorem 3 addresses positive semidefiniteness in all $*$-representations of a C^*-algebra, Proposition 6 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 positive on nonzero hermitian squares is a faithful state, the analogs of these conclusions for O^*-algebras fail (hence the more restricted setup for Proposition 6 is required). Finally, Proposition 6 does not admit a part (iv) as in Theorem 3. In fact, a direct unbounded analog of Theorem 3 fails in this aspect. This is shown in [SW24], and we present a streamlined self-contained example in Subsection 3.2.1 below.

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

Example 7. Consider the Weyl algebra $\mathcal{W} = \mathbb{C}\langle x, y : xy - yx = 1\rangle$ with $x^\star = -x$ and $y^\star = y$. 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 $Xs = \frac{\mathrm{d}}{\mathrm{d}t}s$ 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 $\mathcal{W} = \mathbb{C}\langle a, a^\star : aa^\star - a^\star a = 1\rangle$ 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 Proposition 6, $f(X,Y)$ 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 $\frac{\mathrm{d}}{\mathrm{d}t_1}, \dots, \frac{\mathrm{d}}{\mathrm{d}t_n}$ and multiplication operators $t_1, \dots, t_n$. Its cyclic unit vector is $\pi^{-\frac{n}{4}} e^{-\frac{t_1^2+\cdots+t_n^2}{2}}$.

Example 8. Consider the representation of $\mathbb{C}[x_1,\dots,x_n]$ 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

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

Again, let us view ϕ as a functional on the $\star$-algebra $\mathbb{C}[x_1,\dots,x_n]$, and let $f \in \mathbb{R}[x_1,\dots,x_n]$. Observe that f is nonnegative on $\mathbb{R}^n$ if and only if $f(X_1,\dots,X_n)$ 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 $h \in \mathbb{C}[x_1,\dots,x_n]$. Thus, $f \geq 0$ on $\mathbb{R}^n$ if and only if $\phi(h^2 f) \geq 0$ for all $h \in \mathbb{R}[x_1,\dots,x_n]$ by Proposition 6.

3.2.1 A pushforward counterexample

In this subsection we give an example to show that Proposition 6 does not admit a part (iv) as 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 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 8. 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

$$\begin{aligned} m_n &= \int_{\mathbb{R}} q(t)(t-1)^{6n} e^{-t^2} \,\mathrm{d}t \\ &= \int_0^\infty \left(q(y^{\frac{1}{6}}+1) e^{-2y^{\frac{1}{6}}} + q(-y^{\frac{1}{6}}+1) e^{2y^{\frac{1}{6}}} \right) y^n e^{-y^{\frac{1}{3}}-1} \frac{y^{-\frac{5}{6}}}{6} \,\mathrm{d}y \\ &= \frac{1}{3e} \int_0^\infty \tilde{q}(y) y^{n-\frac{5}{6}} e^{-y^{\frac{1}{3}}} \,\mathrm{d}y, \end{aligned}$$

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

$$\int_0^\infty \Big(\cos\big(\sqrt{3}y^{\frac13}\big)-\sqrt{3}\sin\big(\sqrt{3}y^{\frac13}\big)\Big)y^{n-\frac56}e^{-y^{\frac13}}\,\mathrm{d}y=0$$

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

$$\begin{aligned}\int_0^\infty \tilde{q}(y)y^{n-\frac56}e^{-y^{\frac13}}\,\mathrm{d}y &= \int_0^\infty \Big(\cos\big(2\sqrt{3}y^{\frac13}\big)-\sqrt{3}\sin\big(2\sqrt{3}y^{\frac13}\big)\Big)y^{n-\frac56}e^{-2y^{\frac13}}\,\mathrm{d}y\\ &= 2^{\frac56-n}\int_0^\infty \Big(\cos\big(2\sqrt{3}y^{\frac13}\big)-\sqrt{3}\sin\big(2\sqrt{3}y^{\frac13}\big)\Big)(2y)^{n-\frac56}e^{-2y^{\frac13}}\,\mathrm{d}y=0,\end{aligned}$$

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,

$$\begin{aligned}\phi\big(p(f)^2f\big) &= \int_{\mathbb{R}} p\big((t-1)^6-\varepsilon\big)^2\big((t-1)^6-\varepsilon\big)\frac{e^{-t^2}}{\sqrt{\pi}}\,\mathrm{d}t\\ &= \int_{\mathbb{R}} p\big((t-1)^6-\varepsilon\big)^2\big((t-1)^6-\varepsilon+\eta q(t)\big)\frac{e^{-t^2}}{\sqrt{\pi}}\,\mathrm{d}t\geq 0,\end{aligned}$$

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

3.3 Complete hierarchies of upper bounds

Let $\mathcal{A}$ be a C^*-algebra with a finite generating set S. Impose an order on S, and let S_d be the list of $*$-words in S of length at most d, ordered degree-lexicographically. To a state ϕ on $\mathcal{A}$, $d\in\mathbb{N}$ and $f=f^*\in\mathcal{A}$ we assign the moment matrix

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

In the special case $S=\{f\}$, write

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

for $k\geq 0$. In the next corollary 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 $\sigma_{\min}(f)=\sup\{\alpha\in\mathbb{R}\colon f-\alpha 1\succeq 0\}$.

Corollary 9. *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 $f=f^*\in\mathbb{C}\langle S\rangle$ and $d\in\mathbb{N}$ denote*

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

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 $(\eta_d)_d$ can be viewed as the noncommutative analogues of the sequences recalled in (2) and (4), of upper bounds for standard polynomial optimization from [Las11b] and [Las21], respectively. At a given relaxation order d computing either λ_d or η_d boils down to solving a generalized eigenvalue problem.

Similarly, Proposition 6 yields the following weak analog of Corollary 9 for unbounded operator algebras.

Corollary 10. *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 $f = f^\star \in \mathcal{O}$ and $d \in \mathbb{N}$ denote*

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

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

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

Given a self-adjoint element f of a finitely generated C^*-algebra $\mathcal{A}$, Corollary 9 gives two sequences of generalized eigenvalue problems whose solutions converge to the minimum of f in $\mathcal{A}$, 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 10.

4 Bell inequalities

Now we apply the above framework to obtain lower bounds for maximal violation levels for Bell inequalities. One particularly famous Bell inequality is the CHSH inequality of [CHSH69], where the setting is a quantum system consisting of two measurements for each party, each with the two outcomes ± 1. The measurements can be modeled by four unitary operators x_1, x_2, y_1, y_2 satisfying $x_i^2 = 1 = y_j^2$. Since we are interested in the non-local behavior of our quantum system, we impose the additional constraint that the operators x_i's act on one Hilbert space, and y_j's act on another Hilbert space. The maximum violation of CHSH corresponds to $-\sigma_{\min}(f)$, where $f = -x_1 \otimes y_1 - x_1 \otimes y_2 - x_2 \otimes y_1 + x_2 \otimes y_2$ (acting on the tensor product of Hilbert spaces) under the above unitary/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 (quadratic) polynomial f in hermitian unitaries[1] $x_1, \dots, x_m$ and $y_1, \dots y_n$, where the x_i's commute with the y_j's, such that f is positive semidefinite in the separable C^*-algebra $\mathrm{C}^*_{\text{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\text{full}}(\mathbb{Z}^{\star n})$. The analysis of positivity in this C^*-algebra depends on m and n, as follows.

Proposition 11. *Let $m, n \in \mathbb{N}$, and $G = \mathbb{Z}_2^{\star m} \times \mathbb{Z}_2^{\star n}$. The following holds.*

(a) *G is amenable if and only if $m, n \le 2$.*

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

(c) *If $m \ge 3$ or $n \ge 3$, 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 i^{th} free factor, does not attain its spectral minimum in $\mathrm{C}^*_{\text{red}}(G)$.*

Proof. (a) ($\Rightarrow$) 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), so no group containing $\mathbb{Z}_2 \star \mathbb{Z}_2 \star \mathbb{Z}_2$ can be amenable.

[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 hermitian unitaries.

($\Leftarrow$) If $n, m \le 2$, then G has subexponential growth (concretely, is finite if $m = n = 1$, has linear growth if only one of m, n equals 2, and quadratic growth if $m = n = 2$), and is therefore amenable, see [Tak03, Theorem XIII.4.7] or [Jus22, Section 2.6].

(b) Follows by (a) and [Tak03, Theorem XIII.4.6].

(c) If $m \ge 3$ or $n \ge 3$, then G is not amenable by (a). Then 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 Remark 5. ∎

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

4.1 $m, n \le 2$

In this case, the algebra $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ is isomorphic to $\mathrm{C}^*_{\mathrm{red}}(G)$ by Proposition 11. On $\mathrm{C}^*_{\mathrm{red}}(G)$, there is the canonical faithful state τ given by

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

as in Example 4(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 $u, v \in G$ of length at most d, with the (u, v)-entry equal to $\tau(u^* h v)$. 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 9 implies that $(\lambda_d)_d$ converges to the minimum of f in $\mathrm{C}^*_{\mathrm{red}}(G)$, and thus $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$.

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

If $m \ge 3$ or $n \ge 3$, there exists $f = f^* \in \mathbb{C}[G]$ whose minimum $\sigma_{\min}(f)$ in $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star m}) \otimes_{\min} \mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}^{\star n})$ is strictly lower of the limit of the hierarchy (7). Our strategy to obtain upper bounds converging to $\sigma_{\min}(f)$ is to rely on tensor products of separating sequences (6) from Section 3.3 by parameterizing hermitian unitaries by unitaries and signatures, i.e., by writing each hermitian unitary X_i of size d as $X_i = U_i \begin{bmatrix} \mathbf{I}_{r_i} & 0 \\ 0 & -\mathbf{I}_{d-r_i} \end{bmatrix} U_i^*$ for some $r_i \le d$ and $U_i \in \mathrm{U}_d(\mathbb{C})$. It turns out that it is sufficient to consider only X_i of even size $2d$ with $r_i = d$. One can then consider the state that on a word w in $x_1, \dots, x_n$ evaluates as

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

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 9. To justify the above strategy, we require the following auxiliary statement.

Proposition 12. *Let $f = f^*$ be a polynomial in $m+n$ noncommuting variables $x_1, \dots, x_m, y_1, \dots, y_n$, and let $\sigma_{\min}(f)$ denote the minimum of the spectrum of the canonical image of f in $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m}) \otimes_{\min}$*

$\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$. *Then*

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

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 $\le$ 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 $k\ge d+\max_i|\operatorname{tr}X_i|, e+\max_j|\operatorname{tr}Y_j|$ be 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 $k\times k$ hermitian unitaries $X_i'=X_i\oplus D_i, Y_j'=Y_j\oplus E_j$ satisfy $\operatorname{tr}X_i'=\operatorname{tr}Y_j'=0$. Clearly,

$$\operatorname{mineig} f(X_i\otimes I, I\otimes Y_j)\ge \operatorname{mineig} f(X_i'\otimes I, I\otimes Y_j')$$

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

Note that every $X=X^*\in\mathrm{U}_{2d}(\mathbb{C})$ with $\operatorname{tr}X=0$ is unitarily equivalent to $\left(\begin{smallmatrix} I & 0\\ 0 & -I\end{smallmatrix}\right)$ with $d\times d$ blocks. In analogy with Example 4(5), Proposition 12 implies that

$$\begin{aligned}\psi_d(u\otimes v) = \frac{1}{4d^2}&\left(\int_{U\in\mathrm{U}_{2d}(\mathbb{C})^m} \operatorname{tr} u(U_1SU_1^*,\dots,U_nSU_n^*)\,\mathrm{d}U\right)\\ &\cdot\left(\int_{V\in\mathrm{U}_{2d}(\mathbb{C})^n} \operatorname{tr} v(V_1SV_1^*,\dots,V_mSV_m^*)\,\mathrm{d}V\right)\end{aligned} \tag{9}$$

is a separating sequence of states for $\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star m})\otimes_{\min}\mathrm{C}^*_{\mathrm{full}}(\mathbb{Z}_2^{\star n})$. By Corollary 9, this separating sequence gives rise to a hierarchy of generalized eigenvalue problems whose solutions converge to $\sigma_{\min}(f)$.

5 Numerical examples

Our experiments are performed with Mathematica 13, together with the NCAlgebra package [HdO24] to handle noncommutative polynomials. All results were obtained on an Intel Xeon(R) E-2176M CPU (2.70GHz x 6) with 64Gb of RAM.

5.1 Bell inequalities

Example 13. We consider the CHSH inequality, already mentioned at the beginning of Section 4, where $f=x_1+y_1-x_1y_1-x_1y_2-x_2y_1+x_2y_2$, and the four operators x_1,x_2,y_1,y_2 satisfy $x_i^2=1=y_j^2$ and $x_iy_j=y_jx_i$. The minimal eigenvalue of f is known to be $\sigma_{\min}(f)=(-1-\sqrt{2})/2\simeq-1.207$. With the canonical faithful state τ defined in Section 4.1 and the hierarchy from (7), we report on Figure 1 the values of λ_d for $d=1,\dots,20$. The corresponding computation time is 6 hours. The empirical convergence behavior of the sequence seems to match with the theoretical minimal eigenvalue. The displayed dotted curve is the function $d\mapsto\sigma_{\min}(f)+0.7d^{-1.46}$, so for this particular example we conjecture a heuristic estimate of $O(d^{-1.46})$ for the convergence rate.

For comparison purpose, we also considered the separating state sequence from Section 4.2, given in (9). Preliminary computation outcomes based on the `IntU` Mathematica library by [PM17] are the upper bounds $(\lambda_1, \lambda_2) = (-0.854, -1.016)$, obtained in a few hours. Therefore, one likely needs to be able to efficiently compute quite a few steps before one gets close to the actual value. Further work directions include a more careful algorithmic implementation towards this goal.

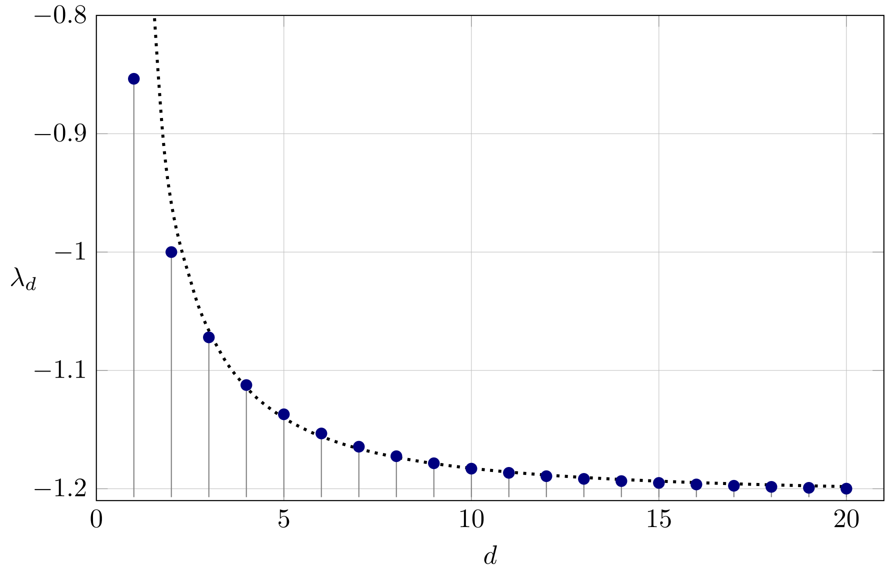

Figure 1: Values λ_d for $d \leq 20$ in Example 13

5.2 Weyl algebras

Example 14. 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 7. After applying the change of variable $a = \frac{x+y}{\sqrt{2}}$ one has $\mathcal{W} = \mathbb{C}\langle a, a^\star \colon aa^\star - a^\star a = 1\rangle$, and one considers the faithful vector state ϕ:

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

For $h \in \mathcal{W}$ let $\mathbf{M}_d(h\,\phi)$ be the $(d+1)^2 \times (d+1)^2$ matrix indexed by $a^{*m}a^n$ for $m, n \leq d$, whose $(a^{*k}a^\ell, a^{*m}a^n)$-entry equals $\phi(a^{*\ell}a^k h\, a^{*n}a^m)$. Given $f \in \mathcal{W}$, Example 7 and Corollary 10 show that the values

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

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 variable $a = \frac{x+y}{\sqrt{2}}$, one has $f_1 = 1 + 8a^*a + 4{a^*}^2a^2$, 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].

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 $\beta = 1$.

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 $\sigma_{\min}(f_2) \simeq 1.392352$.

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 15. 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 8 and Corollary 10 show that the values

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

form a decreasing 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 2 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 is the function $d \mapsto \sigma_{\min}(f) + 3d^{-0.65}$, so for this particular example we conjecture a heuristic estimate of $O(d^{-0.65})$ for the convergence rate.

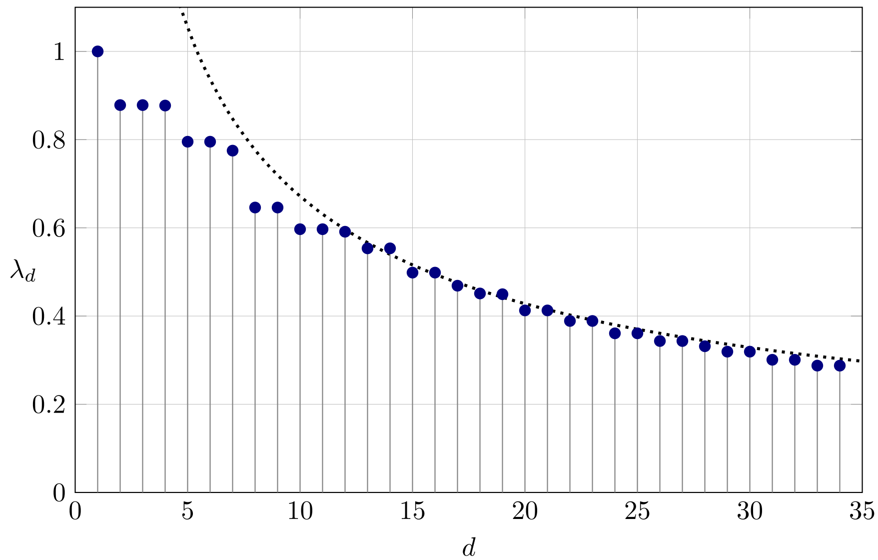

Figure 2: Values λ_d for $d \leq 34$ in Example 15

5.4 Optimizing an exponential function

Example 16. As in [AGN24, § V-B], consider the spectral minimum of $\exp(X_0X_1 + X_1X_0)$ for arbitrary orthogonal projections X_0, X_1 on a Hilbert space.

The universal C^*-algebra

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

is isomorphic to $\mathrm{C}^*_{\text{full}}(\mathbb{Z}_2 \star \mathbb{Z}_2) = \mathrm{C}^*_{\text{red}}(\mathbb{Z}_2 \star \mathbb{Z}_2)$ (via $x_j \mapsto 2x_j - 1 =: e_j$), and thus admits the canonical tracial state τ as in Example 4(a).

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 $[0, 2\pi]$,

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

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 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 $r \in \mathbb{N}$,

$$\pi\big((e_0e_1)^r\big) = \begin{bmatrix} \cos(r\phi) & \sin(r\phi) \\ -\sin(r\phi) & \cos(r\phi) \end{bmatrix},$$

whence

$$\tau'\big((e_0e_1)^r\big) = \frac{1}{2\pi}\int_0^{2\pi} \cos(r\phi)\,\mathrm{d}\phi = \begin{cases} 1 & r = 0, \\ 0 & \text{otherwise.} \end{cases}$$

Similarly, $\tau'\big((e_0e_1)^r e_0\big) = 0$ 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,

$$\pi\big((x_0x_1)^r\big) = \begin{bmatrix} \frac{1}{2^r}(1+\cos(\phi))^r & * \\ 0 & 0 \end{bmatrix},$$

so

$$t_{2r} = \tau\big((x_0x_1)^r\big) = \tau'\big((x_0x_1)^r\big) = \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{2^r}(1+\cos(\phi))^r\,\mathrm{d}\phi = \frac{\Gamma\left(r+\frac{1}{2}\right)}{2\sqrt{\pi}\,\Gamma(r+1)} = \frac{\Gamma\left(r+\frac{1}{2}\right)}{2\sqrt{\pi}\,r!}.$$

Let $f = e^{x_0x_1+x_1x_0}$. 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

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

so

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

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

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

for $d \in \mathbb{N}$. By Corollary 9,

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

is a decreasing sequence whose limit is the spectral minimum of $\exp(X_0X_1 + X_1X_0)$ for orthogonal projections X_0, X_1.

Figure 16 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 is the function $d \mapsto \sigma_{\min}(f) + 0.4d^{-1.58}$, so for this particular example we conjecture a heuristic estimate of $O(d^{-1.58})$ for the convergence rate. The minimum in this example is $\sigma_{\min}(f) = \exp(-\frac{1}{4}) \approx 0.778801$.

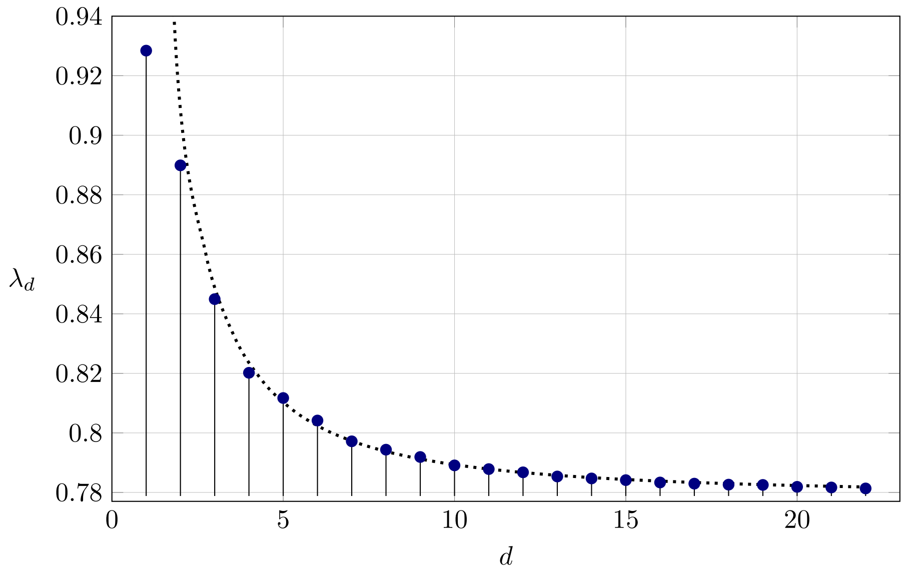

Figure 3: Values λ_d for $d \leq 22$ in Example 16

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 case, while there is no empirical evidence that the Lasserre hierarchy of upper bounds could outperform classical numerical schemes such as brute-force sampling methods based on Monte-Carlo or local optimization solvers based on gradient descent, it turns out that the asymptotic behavior of the upper bound hierarchy has been better understood than for the lower bound hierarchy. In [dKLS16], the authors obtain convergence rates which often match practical experiments and are no worse than $O(1/\sqrt{d})$, where d is the relaxation order in the hierarchy. On some specific sets this convergence rate has been improved to $O(1/d^2)$, e.g., for the box $[-1,1]^n$ by [DKHL17] and for the sphere by [dKL22]. Recently, similar convergence rates could be obtained by [Slo22] for the standard hierarchy of lower bounds by combining upper bound rates with an elegant use of Christoffel-Darboux kernels; see [LPP22] for a recent survey on these kernels. 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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