

A SEMIDEFINITE HIERARCHY FOR CONTAINMENT OF SPECTRAHEDRA

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ABSTRACT. A spectrahedron is the positivity region of a linear matrix pencil and thus the feasible set of a semidefinite program. We propose and study a hierarchy of sufficient semidefinite conditions to certify the containment of a spectrahedron in another one. This approach comes from applying a moment relaxation to a suitable polynomial optimization formulation. The hierarchical criterion is stronger than a solitary semidefinite criterion discussed earlier by Helton, Klep, and McCullough as well as by the authors. Moreover, several exactness results for the solitary criterion can be brought forward to the hierarchical approach.

The hierarchy also applies to the (equivalent) question of checking whether a map between matrix (sub-)spaces is positive. In this context, the solitary criterion checks whether the map is completely positive, and thus our results provide a hierarchy between positivity and complete positivity.

1. INTRODUCTION

Containment problems of convex sets belong to the classical problems in convex geometry (see, e.g., Gritzmann and Klee for the containment of polytopes [15], Freund and Orlin for containment problems of balls in balls [10], or Mangasarian for containment of convex sets in reverse-convex sets [32]).

In this paper, we consider the containment problem for spectrahedra using the following common notation. Let \mathcal{S}_k be the set of real symmetric $k \times k$ -matrices, \mathcal{S}_k^+ be the set of positive semidefinite $k \times k$ -matrices, and $\mathcal{S}_k[x]$ be the set of symmetric $k \times k$ -matrices with polynomial entries in $x = (x_1, \dots, x_n)$. For $A_0, \dots, A_n \in \mathcal{S}_k$, denote by $A(x)$ the *linear (matrix) pencil* $A(x) = A_0 + x_1 A_1 + \dots + x_n A_n \in \mathcal{S}_k[x]$. The set

$$(1.1) \quad S_A = \{x \in \mathbb{R}^n : A(x) \succeq 0\}$$

is called a *spectrahedron*, where $A(x) \succeq 0$ denotes positive semidefiniteness of the matrix $A(x)$. Our work is intrinsically motivated by the fact that spectrahedra have become an important class of non-polyhedral sets due to the availability of fast semidefinite programming solvers. See [6, 7, 11, 18, 33] for general background on spectrahedra, and their significance in optimization and convex algebraic geometry. Spectrahedra can be used to represent observables in quantum information theory [41]. From an application point of view, interest in non-polyhedral, and thus particularly semidefinite, set containment is stimulated by non-polyhedral knowledge based data classification (see [23, 32], for semidefinite classifiers see [24]).

Given two linear pencils $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$, the containment problem for spectrahedra is to decide whether $S_A \subseteq S_B$. This problem is co-NP-hard [4, 25].

The study of algorithmic approaches and relaxations has been initiated by Ben-Tal and Nemirovski [4] who investigated the case where S_A is a cube (“matrix cube problem”). Helton, Klep, and McCullough [17] studied containment problems of matricial positivity domains (which live in infinite-dimensional spaces), and from this they derive a *semi-definite* sufficient criterion for deciding containment of spectrahedra. In [25], the authors of the present paper provided a streamlined presentation of the results on spectrahedral containment in [17] and showed that in several cases the sufficient criterion is exact.

From an operator algebra point of view (such as in [17, 26]), this semidefinite feasibility condition states that a natural linear map Φ_{AB} between the subspaces $\mathcal{A} = \text{span}(A_0, \dots, A_n)$ and $\mathcal{B} = \text{span}(B_0, \dots, B_n)$ is *completely positive* (as defined in Section 4.1). These maps also appear in the context of Positivstellensätze in non-commuting variables; see [16]. Building upon these results, in the current paper we go one step further, presenting a hierarchy of monotone improving sufficient semidefinite optimization problems to decide the containment question.

Our point of departure is to formulate the containment problem in terms of polynomial matrix inequalities (PMI). We use common relaxation techniques (by Kojima [27], Hol and Scherer [21] as well as Henrion and Lasserre [20]) to derive a (sufficient) semidefinite hierarchy for the containment problem. The semidefinite hierarchy provides a much more comprehensive approach towards the containment problems than the aforementioned sufficient criterion (see Theorem 4.8). We also discuss a variant of the semidefinite hierarchy which avoids additional variables (see Section 3.3).

Main contributions. 1. Based on polynomial matrix inequalities, we provide a hierarchy of sufficient semidefinite criteria for the containment problem and prove that the sequence of optimal values converges to the optimal value of the underlying polynomial optimization problem; see Theorem 3.3.

2. Any relaxation step of the hierarchy yields a sufficient criterion for the containment problem. We prove that each of these sufficient criteria is at least as powerful as the one in [17, 25], in the sense that whenever the criterion of [17, 25] is satisfied, then also the criterion from any of the relaxation steps of the hierarchy is satisfied; see Theorem 4.8. In particular, this already holds for the criterion coming from the initial relaxation step. This allows to carry all exactness results from [25] forward to our new hierarchical approach; see Corollaries 4.11 and 4.12.

3. Application of the hierarchy to the problem of deciding whether a linear map between matrix subspaces is positive gives a monotone semidefinite hierarchy of sufficient criteria for this problem.

4. We demonstrate the effectiveness of the approach by providing numerical results for several containment problems and radii computations.

We remark that the containment question is intimately linked to the computation of inner and outer radii of convex sets. (See Gritzmann and Klee [13, 14] for the polytope case). Moreover, Bhardwaj, Rostalski, and Sanyal [5] study the related question of whether a spectrahedron is a polytope. In [12], Gouveia, Robinson, and Thomas reduced the question of computing the positive semidefinite rank of nonnegative matrices to a containment problem involving projections of spectrahedra.

The paper is structured as follows. In Section 2, we collect some notations and concepts on spectrahedra and polynomial matrix inequalities. The semidefinite hierarchy, as well as a variant avoiding additional variables, is introduced in Section 3. In Section 4, we connect the hierarchy to (complete) positivity of operators and the sufficient semidefinite criteria from [17, 25]. Section 5 discusses applications of radii computations and provides numerical results.

2. PRELIMINARIES

Throughout, general matrix polynomials will be denoted by $G(x) \in \mathcal{S}_k[x]$, while linear matrix pencils will usually be denoted by $A(x) \in \mathcal{S}_k[x]$ or $B(x) \in \mathcal{S}_l[x]$. Let I_n abbreviate the $n \times n$ identity matrix, and let E_{ij} denote the matrix with a one in position (i, j) and zeros elsewhere. By $\mathbb{B}_r(p)$, we denote the (closed) Euclidean ball with center p and radius $r > 0$.

2.1. Spectrahedra and semidefinite programming. Given a linear pencil

$$(2.1) \quad A(x) = A_0 + \sum_{p=1}^n x_p A_p \in \mathcal{S}_k[x] \quad \text{with } A_p = (a_{ij}^p), \quad 0 \leq p \leq n,$$

the spectrahedron $S_A = \{x \in \mathbb{R}^n : A(x) \succeq 0\}$ contains the origin if and only if A_0 is positive semidefinite. Since the class of spectrahedra is closed under translation, this can always be achieved (assuming that S_A is nonempty). Indeed, there exists a point $x' \in \mathbb{R}^n$ such that $A(x') \succeq 0$ if and only if the origin is contained in the set $\{x \in \mathbb{R}^n : A(x + x') \succeq 0\}$. In particular, the constant term in the linear pencil $A'(x) = A(x + x')$ is positive semidefinite.

The equivalence between positive definiteness of A_0 and the origin being an interior point is not true. Moreover, in general, the interior of S_A does not coincide with the positive definiteness region of the pencil. However, if the spectrahedron S_A has nonempty interior (or, equivalently, S_A is full-dimensional), then there exists a *reduced* linear pencil that is positive definite exactly on the interior of S_A .

Proposition 2.1 ([11, Corollary 5]). *Let $S_A = \{x \in \mathbb{R}^n : A(x) \succeq 0\}$ be full-dimensional and let N be the intersection of the nullspaces of A_i , $i = 0, \dots, n$. If V is a basis of the orthogonal complement of N , then $S_A = \{x \in \mathbb{R}^n : V^T A(x) V \succeq 0\}$ and the interior of S_A is $\text{int}(S_A) = \{x \in \mathbb{R}^n : V^T A(x) V \succ 0\}$.*

Furthermore, the spectrahedron S_A contains the origin in its interior if and only if there is a linear pencil $A'(x)$ with the same positivity domain such that $A'_0 = I_k$; see [19]. To simplify notation, we sometimes assume that $A(x)$ is of this form and refer to it as a *monic* linear pencil, i.e., $A_0 = I_k$.

In addition, we occasionally assume the matrices A_1, \dots, A_n to be linearly independent. This assumption is not too restrictive. In order to see this, denote by $\tilde{A}(x) = A(x) - A_0$ the pure-linear part of the linear pencil $A(x)$. Recall the well-known fact that the *lineality space* L_A of a spectrahedron S_A , i.e., the largest linear subspace contained in S_A , is the set $L_A = \{x \in \mathbb{R}^n : \tilde{A}(x) = 0\}$; see [11, Lemma 3]. Obviously, if the coefficient matrices A_1, \dots, A_n are linearly independent, then the lineality space is zero-dimensional, i.e., $L_A = \{0\}$. In particular, this is the case whenever the spectrahedron S_A is bounded

(and $A_0 \succeq 0$); see [17, Proposition 2.6]. Conversely, if there are linear dependencies in the coefficient matrices, then we can simply reduce the containment problem to lower dimensions.

Proposition 2.2. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils such that S_A is non-empty.*

- (1) $L_A = \{0\}$ if and only if A_1, \dots, A_n are linearly independent.
- (2) If $S_A \subseteq S_B$, then $L_A \subseteq L_B$.
- (3) If $L_A \subseteq L_B$, then $S_A \subseteq S_B$ holds if and only if $S_{A'} \subseteq S_{B'}$ holds, where $S_{A'} = S_A \cap L_A^\perp$ and $S_{B'} = S_B \cap L_A^\perp$.

To prove the Proposition, we need a result concerning the lineality space of a closed convex set.

Lemma 2.3. [40, Theorem 2.5.8] *Let S be a non-empty closed convex set in \mathbb{R}^n with lineality space L . Then $S = L + (S \cap L^\perp)$ and the convex set $S \cap L^\perp$ contains no lines.*

Proof. (of Proposition 2.2)

To (1): This follows directly from $L_A = \{x \in \mathbb{R}^n : \tilde{A}(x) = 0\}$ and the definition of linear independence.

To (2): If $L_A = \{0\}$, then $L_A \subseteq L_B$ is obviously true. Therefore, assume $L_A \neq \{0\}$. Let $\bar{x} \in S_A \subseteq S_B$ and $0 \neq x \in L_A$. As above, denote by $\tilde{B}(x) = B(x) - B_0 = \sum_{p=1}^n x_p B_p$ the pure-linear part of $B(x)$. Then $A(\bar{x} + tx) \succeq 0$ for all $t \in \mathbb{R}$ and hence $B(\bar{x}) \pm t\tilde{B}(x) = B(\bar{x} \pm tx) \succeq 0$ for all $t \in \mathbb{R}$. Consequently, $\pm\tilde{B}(x) \succeq 0$, i.e., $\tilde{B}(x) = 0$. Thus the linear subspace $\text{span } x$ is contained in L_B . Since $0 \neq x \in L_A$ was arbitrary and L_B is a linear subspace, we have $L_A \subseteq L_B$.

To (3): Assume first $S_A \subseteq S_B$ holds. Then $S_{A'} = S_A \cap L_A^\perp \subseteq S_B \cap L_A^\perp = S_{B'}$. For the converse, note that $S_A = L_A + S_{A'}$. Let $x \in S_A$. Then $x = x_1 + x_2$ with $x_1 \in L_A$ and $x_2 \in S_{A'}$. Since $x_1 \in L_A \subseteq L_B$ and $x_2 \in S_{A'} \subseteq S_{B'} \subseteq S_B$, we have $x \in L_B + S_B = S_B$. \square

A (linear) *semidefinite program* (SDP) is an optimization problem where one optimizes a linear objective function $c^T x$ over a spectrahedron, $\inf \{c^T x : A(x) \succeq 0\}$. A *semidefinite feasibility problem* (SDFP) is the decision problem of deciding whether for a given linear pencil $A(x)$ the spectrahedron S_A is nonempty. While SDPs (with rational input data) can be approximated in polynomial time (see [9]), the complexity of SDFP is open. The best known results are contained in [35]. In practice, however, SDFPs can be solved efficiently by semidefinite programming.

2.2. Polynomial matrix inequalities. Problems involving a polynomial objective function and positive semidefinite constraints on matrix polynomials are called *polynomial matrix inequality* (PMI) problems and can be written in the following standard form.

$$(2.2) \quad \begin{array}{ll} \inf & f(x) \\ \text{s.t.} & G(x) \succeq 0, \end{array}$$

where $f(x) \in \mathbb{R}[x]$ and $G(x) \in \mathcal{S}_k[x]$, not necessarily linear, for $x = (x_1, \dots, x_n)$.

Hol and Scherer [21], and Kojima [27] introduced sums of squares relaxations for PMIs, leading to semidefinite programming relaxations of the original problem. Here we focus mainly on the dual viewpoint of moment relaxations, as exhibited by Henrion and Lasserre [20]. As in Lasserre’s moment method for polynomial optimization [28], the basic idea is to linearize all polynomials by introducing a new variable for each monomial. The relations among the monomials give semidefinite conditions on the moment matrices.

As discussed in [20], directly linearizing the positive semidefiniteness condition (2.2) can lead to relaxations that use a relatively small number of variables. To formalize this, let $[x]$ be the monomial basis of $\mathbb{R}[x]$ and let $y = \{y_\alpha\}_{\alpha \in \mathbb{N}^n}$ be a real-valued sequence indexed in the basis $[x]$. A polynomial $p(x) \in \mathbb{R}[x]$ can be identified by its vector of coefficients \vec{p} in the basis $[x]$. By $[x]_t$ we denote the truncated basis containing only monomials of degree at most t . For the linearization operation, consider the operator L_y defined by the linear mapping $p \mapsto L_y(p) = \langle \vec{p}, y \rangle$.

Let $M(y)$ be the moment matrix defined by $[M(y)]_{\alpha,\beta} = L_y([x][x]^T)_{\alpha,\beta} = y_{\alpha+\beta}$. $M_t(y)$ denotes the truncated moment matrix that contains only entries $[M(y)]_{\alpha,\beta}$ with $|\alpha|, |\beta| \leq t$.

The positive semidefiniteness constraint on a matrix polynomial $G(x) \in \mathcal{S}_k[x]$ can be modelled by so called *localizing matrices* (which for 1×1 -matrices specialize to the usual localizing matrices within Lasserre’s relaxation for polynomial optimization [28]). The truncated localizing matrix $M_t(Gy)$ is the block matrix obtained by

$$[M_t(Gy)]_{\alpha,\beta} = L_y([x]_t[x]_t^T \otimes G(x))_{\alpha,\beta}.$$

We write $M_t(Gy) = L_y([x]_t[x]_t^T \otimes G(x))$ for short. Let d_G be the highest degree of a polynomial appearing in $G(x)$. With this notation only linearization variables coming from monomials of degree at most $2t + d_G$ appear in $M_t(Gy)$.

We arrive at the following hierarchy of semidefinite relaxations for the polynomial optimization problem (2.2),

$$(2.3) \quad \begin{aligned} f_{\text{mom}}^{(t)} &= \inf L_y(f(x)) \\ &\text{s.t. } M_t(y) \succeq 0 \\ &\quad M_{t-\lceil d_G/2 \rceil}(Gy) \succeq 0. \end{aligned}$$

We only use the monomial basis of degree up to $t - \lceil d_G/2 \rceil$ in the last constraint so that only moments coming from variables of degree $2t$ or lower appear in the whole optimization problem. Note that $t = \lceil \max\{d_G, d_f\}/2 \rceil$ is the smallest possible relaxation order, since for smaller t there are unconstrained variables in the objective or the truncated localizing matrix is undefined. We call $t = \lceil \max\{d_G, d_f\}/2 \rceil$ the *initial relaxation order*.

The optimal value of the hierarchy (2.3) converges under mild assumptions to the optimal value of the original problem (2.2). To make this statement precise, we call a matrix polynomial $S(x) \in \mathcal{S}_k[x]$ a *sum of squares* (or *sos-matrix*) if it has a decomposition $S(x) = U(x)U(x)^T$ with $U(x) \in \mathbb{R}^{k \times m}[x]$ for some positive integer m . For $k = 1$, $S(x)$ is called *sos-polynomial*.

Proposition 2.4. [20, Theorem 2.2], see also [21, Theorem 1]. *Let $G(x) \in \mathcal{S}_k[x]$. Assume there exists a polynomial $p(x) = s(x) + \langle S(x), G(x) \rangle$ for some sos-polynomial $s(x) \in \mathbb{R}[x]$*

and some sos-matrix $S(x) \in \mathcal{S}_k[x]$, such that the level set $\{x \in \mathbb{R}^n : p(x) \geq 0\}$ is compact. Then $f_{\text{mom}}^{(t)} \uparrow f^*$ as $t \rightarrow \infty$ in the semidefinite hierarchy (2.3).

3. A (SUFFICIENT) SEMIDEFINITE HIERARCHY

Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be two linear pencils. In this section, we provide an optimization formulation to decide the question of whether the spectrahedron S_A is contained in S_B . Using a PMI formulation of the containment problem, we first deduce a sufficient semidefinite hierarchy and prove the convergence of the hierarchy (Theorem 3.3). Afterwards, we state a second, in fact highly related, approach based on a quantified semidefinite program; see Subsection 3.3.

3.1. An optimization approach to decide containment of spectrahedra. Clearly, S_A is contained in S_B if and only if $A(x) \succeq 0$ implies the positive semidefiniteness of $B(x)$. By definition, $B(x) \succeq 0$ for arbitrary but fixed $x \in \mathbb{R}^n$ is equivalent to the nonnegativity of the polynomial $z^T B(x) z$ in the variables $z = (z_1, \dots, z_l)$. Thus, S_A is contained in S_B if and only if the infimum μ of the degree 3 polynomial $z^T B(x) z$ in (x, z) over the spectrahedron $S_A \times \mathbb{R}^l$ is nonnegative. Imposing a normalization condition on z , we arrive at the following formulation.

Proposition 3.1. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils with $S_A \neq \emptyset$, and let $g_r(z) = z^T z - r^2$, $g^R(z) = R^2 - z^T z$ for arbitrary but fixed $0 < r \leq R$. For the polynomial optimization problem*

$$(3.1) \quad \begin{aligned} \mu &= \inf z^T B(x) z \\ \text{s.t. } G_A(x, z) &:= \text{diag}(A(x), g_r(z), g^R(z)) \succeq 0 \end{aligned}$$

the following implications are true,

$$\begin{aligned} \mu > 0 &\Rightarrow S_A \subseteq \text{int } S_B, \\ \mu = 0 &\Rightarrow S_A \subseteq S_B, \\ \mu < 0 &\Leftrightarrow \exists x \in S_A : B(x) \not\succeq 0. \end{aligned}$$

If the pencil $B(x)$ is reduced in the sense of Proposition 2.1, $\mu = 0$ implies that the spectrahedra touch at the boundary.

A natural choice of the parameters r and R is to set both to 1. In this case, the optimal value of the optimization problem equals the smallest eigenvalue of any matrix in the set $\{B(x) : x \in S_A\}$. Other choices result in an optimal value that is scaled by R^2 in the case $\mu < 0$ and by r^2 in the case $\mu > 0$. As our numerical computations in Section 5 show, the problem, or, more precisely, its relaxation defined in Section 3.2 is numerically ill-conditioned if we chose $r = R$ and becomes more tractable for $r < R$.

In applications, it is advisable to use reduced pencils. The reduced pencil can be computed by the methods in [11] and makes the numerical computations described below better conditioned. Not only do we expect a strictly positive objective value whenever $S_A \subseteq \text{int } S_B$, the reduced pencil is also of smaller size.

Proof (of Proposition 3.1). Denote by $\mathbb{T} = \mathbb{T}_{r,R}(0) = \{z \in \mathbb{R}^l : r^2 \leq z^T z \leq R^2\}$ the annulus defined by the constraints $g_r(z) \geq 0$, $g^R(z) \geq 0$.

We first observe that the existence of an $x \in S_A$ and $z \in \mathbb{R}^l$ with $z^T B(x)z < 0$ implies the existence of a point $z' := R \cdot \frac{z}{\|z\|} \in \mathbb{T}$ with $\|z'\| = R$ and $z'^T B(x)z' < 0$, and thus (x, z') lies in the product of the spectrahedron S_A and the annulus \mathbb{T} .

If $\mu \geq 0$, then clearly $S_A \subseteq S_B$. To deduce the case $\mu > 0$, observe that the boundary ∂S_B of S_B is contained in the set

$$\{x \in \mathbb{R}^n : B(x) \succeq 0, z^T B(x)z = 0 \text{ for some } z \in \mathbb{T}\}.$$

Hence, if the boundaries of S_A and S_B contain a common point \bar{x} , then there exists some \bar{z} such that the objective value of (\bar{x}, \bar{z}) is zero. \square

3.2. Derivation of the hierarchy using moment relaxation methods. Using the framework of moment relaxations for PMIs introduced in Section 2.2, we consider the following semidefinite hierarchy as a relaxation to problem (3.1), providing a semidefinite hierarchy for the containment question. Let y be a real-valued sequence indexed by $[x, z]$, the monomial basis of $\mathbb{R}[x, z] = \mathbb{R}[x_1, \dots, x_n, z_1, \dots, z_l]$. For $t \geq 2$, we obtain the t -th relaxation of the polynomial optimization problem (3.1)

$$(3.2) \quad \begin{aligned} \mu_{\text{mom}}(t) &= \inf L_y(z^T B(x)z) \\ &\text{s.t. } M_t(y) \succeq 0 \\ &\quad M_{t-1}(GAy) \succeq 0. \end{aligned}$$

As described in Subsection 2.2, we only use the monomial basis of degree up to $t - 1$ in the last constraint so that only moments coming from variables of degree $2t$ or lower appear in the whole optimization problem. Note that $t = 2$ is the initial relaxation order, as defined in Section 2.2. By increasing t , additional constraints are added, which implies the following corollary.

Corollary 3.2. *The sequence $\mu_{\text{mom}}(t)$ for $t \geq 2$ is monotone non-decreasing. If for some t^* the condition $\mu_{\text{mom}}(t^*) \geq 0$ is satisfied, then $S_A \subseteq S_B$.*

That is, for any t , the condition $\mu_{\text{mom}}(t) \geq 0$ provides a sufficient criterion for the containment $S_A \subseteq S_B$. In the case when the inner spectrahedron S_A is bounded, the sequence of relaxations is not only monotone non-decreasing, but also converges to the optimal value of the original polynomial optimization problem (3.1), as the next theorem shows.

Theorem 3.3. *Let $A(x) \in \mathcal{S}_k[x]$ be a linear pencil such that the spectrahedron S_A is bounded. Then the optimal value of the moment relaxation (3.2) converges from below to the optimal value of the polynomial optimization problem (3.1), i.e., $\mu_{\text{mom}}(t) \uparrow \mu$ as $t \rightarrow \infty$.*

Proof. By Proposition 2.4, it suffices to show that there exists an sos-polynomial $s(x, z) \in \mathbb{R}[x, z]$ and an sos-matrix $S(x, z) \in \mathcal{S}_{k+2}[x, z]$ defining a polynomial $p(x, z) = s(x, z) +$

$\langle S(x, z), G_A(x, z) \rangle$ such that the level set $\{(x, z) \in \mathbb{R}^{n+l} : p(x, z) \geq 0\}$ is compact. Define the quadratic module

$$M_A = \{t(x) + \langle A(x), T(x) \rangle : t(x) \in \mathbb{R}[x] \text{ sos-polynomial, } T(x) \in \mathcal{S}_k[x] \text{ sos-matrix}\}.$$

As shown in [26, Corollary 2.2.6], the boundedness of S_A is equivalent to the fact that the quadratic module M_A is Archimedean, i.e., there exists a positive integer $N \in \mathbb{N}$ such that $N - x^T x \in M_A$. Thus, by the definition of the quadratic module M_A , there exists an sos-polynomial $t(x) \in \mathbb{R}[x]$ and an sos-matrix $T(x) \in \mathcal{S}_k[x]$ such that

$$N - x^T x = t(x) + \langle T(x), A(x) \rangle.$$

Define $s(x, z) = t(x)$ and $S(x, z) = \text{diag}(T(x), 0, 1)$. Both have the sos-property. Indeed, if $T(x) = U(x)U(x)^T$ is an sos-decomposition of $T(x)$, then $S(x, z) = \text{diag}(T(x), 0, 1) = \text{diag}(U(x), 0, 1) \text{diag}(U(x)^T, 0, 1)$ is one of $S(x, z)$. We get

$$p(x, z) = N - x^T x + R^2 - z^T z = s(x, z) + \langle S(x, z), G_A(x, z) \rangle.$$

Since this polynomial defines the ball of radius $N + R^2$ centered at the origin, $\mathbb{B}_{N+R^2}(0) \subset \mathbb{R}^{n+l}$, the level set is compact. \square

Remark 3.4. Computing a certificate N from the proof of the theorem can again be done by the polynomial semidefinite program (3.1) and its relaxation (3.2). We have a deeper look on this in Section 5.3. In fact, the program stated there computes the circumradius of the spectrahedron S_A , if it is centrally symmetric with respect to the origin.

If the optimal value of the polynomial reformulation (3.1) equals zero, it might lead to numerical issues in the relaxation (3.2) as it requires the computation of an exact value via semidefinite programming. From a geometric point of view this occurs only in somewhat degenerate cases: the spectrahedra touch at the boundary or the determinantal variety of $B(x)$ intersects the interior of the spectrahedron S_A ; if the pencil $B(x)$ is reduced in the sense of Proposition 2.1, the latter case is not possible.

3.3. An alternative formulation. A crucial point in the polynomial optimization approach (3.1) is the introduction of additional variables $z = (z_1, \dots, z_l)$ already in the original, unrelaxed polynomial formulation (see Proposition 3.1). An alternative approach would be to start from the following quantified semidefinite program without additional variables,

$$(3.3) \quad \begin{aligned} \mu &= \sup \lambda \\ \text{s.t. } & B(x) - \lambda I_l \succeq 0 \quad \forall x \in S_A. \end{aligned}$$

By a result on robust polynomial semidefinite programming by Hol and Scherer [36] this class of problems can be solved by an approach based on sum-of-squares matrix polynomials, leading to a hierarchy of the form

$$(3.4) \quad \begin{aligned} \lambda_{\text{sos}}(t) &= \sup \lambda \\ \text{s.t. } & B(x) - \lambda I_l - (\langle S_{i,j}(x), A(x) \rangle)_{i,j=1}^l \text{ sos-matrix} \\ & S(x) = (S_{i,j}(x))_{i,j=1}^l \in \mathcal{S}_{kl}[x] \text{ sos-matrix.} \end{aligned}$$

where $S(x)$ has $l \times l$ blocks of size $k \times k$ with entries of degree at most $2t \geq 0$. Using Theorem 1 and Corollary 1 from [36], we can state the subsequent convergence statement for the sos-relaxation. The proof of this theorem is very similar to the one of Theorem 3.3.

Theorem 3.5. *Let $A(x) \in \mathcal{S}_k[x]$ be a linear pencil such that the spectrahedron S_A is bounded. Then the optimal value of the sos-relaxation (3.4) converges from below to the optimal value of the quantified semidefinite optimization problem (3.3), i.e., $\lambda_{\text{sos}}(t) \uparrow \mu$ as $t \rightarrow \infty$.*

While in the quantified semidefinite program no additional variables $z = (z_1, \dots, z_l)$ are needed, the number of unknowns of the relaxation grows not only in the number of variables n and the relaxation order t , i.e., half the degree of the entries in $S(x)$, but also in the size of both the outer pencil l and the inner pencil k . To be more precise, using the approach of Hol and Scherer, the number of unknowns in the SDP coming from the sos-relaxation is generically

$$1 + \frac{1}{2} \binom{n+t}{t} \cdot \left[k^2 l^2 \binom{n+t}{t} + l^2 \binom{n+t}{t} + kl + l \right] - ml(l+1),$$

where m denotes the number of affine equation constraints arising in the sos-formulation; see [36, Section 5]. In our main approach there are

$$\frac{1}{2} \binom{n+l+t}{t} \left[\binom{n+l+t}{t} - 1 \right]$$

variables. In certain situations with small t (i.e., $t \in \{0, 1\}$), the sos-approach may lead to SDPs with a simpler structure than our main approach. We study this in detail in Section 5.

4. POSITIVITY OF MATRIX MAPS AND THE HIERARCHY FOR CONTAINMENT

In this section, we first review the containment criterion based on complete positivity of operators that was studied in [17, 25]. We then prove that the sufficient criteria coming from our hierarchy of relaxations are at least as strong as the complete positivity criterion by showing that feasibility of the complete positivity criterion implies $\mu \geq 0$ in the initial relaxation step of the semidefinite hierarchy (3.2). From this relation, we get that in some cases already the initial relaxation step gives an exact answer to the containment problem; see Corollaries 4.11 and 4.12.

For the convenience of the reader, we first collect the relevant connections between the containment problem and (complete) positivity of maps between matrix spaces; see Statements 4.2–4.6. Theorem 4.8 gives our main result concerning the containment criterion from [17, 25] and the semidefinite hierarchy.

4.1. (Completely) positive maps. Besides providing a (numerical) answer to the containment question, the semidefinite hierarchy (3.2) is useful to detect positivity of linear maps between (subspaces of) matrix spaces.

The concepts discussed in this subsection can be defined in a much more general setting, using the language of operator theory. See, e.g., [34] for an introduction to positive and completely positive maps on C^* -algebras.

Definition 4.1. Given two linear subspaces $\mathcal{A} \subseteq \mathbb{R}^{k \times k}$ and $\mathcal{B} \subseteq \mathbb{R}^{l \times l}$, a linear map $\Phi : \mathcal{A} \rightarrow \mathcal{B}$ is called *positive* if every positive semidefinite matrix in \mathcal{A} is mapped to a positive semidefinite matrix in \mathcal{B} , i.e., $\Phi(\mathcal{A} \cap \mathcal{S}_k^+) \subseteq \mathcal{B} \cap \mathcal{S}_l^+$.

The map Φ is called *d-positive* if the map $\Phi_d : \mathbb{R}^{d \times d} \otimes \mathcal{A} \rightarrow \mathbb{R}^{d \times d} \otimes \mathcal{B}$, $M \otimes A \mapsto M \otimes \Phi(A)$ is positive, i.e. $(\Phi(A_{ij}))_{i,j=1}^d \in \mathcal{B}^{d \times d} \cap \mathcal{S}_{dl}^+$ for $(A_{ij})_{i,j=1}^d \in \mathcal{A}^{d \times d} \cap \mathcal{S}_{dk}^+$.

Finally, Φ is called *completely positive* if Φ_d is positive for all positive integers d .

Naturally, every d -positive map is e -positive for all positive integers $e \leq d$. Provided that \mathcal{A} contains a positive definite matrix, complete positivity of Φ is equivalent to k -positivity; see [34, Theorem 6.1]. Interestingly, in this situation every completely positive map does have a completely positive extension to the full matrix space and can therefore be represented by a positive semidefinite matrix. This is well known in the general setting of C^* -algebras and persists in our real setting.

Proposition 4.2 ([34, Theorem 6.2.]). *Let $\mathcal{A} \subseteq \mathbb{R}^{k \times k}$ be a linear subspace containing a positive definite matrix, then each completely positive map $\Phi : \mathcal{A} \rightarrow \mathbb{R}^{l \times l}$ has an extension to a completely positive map $\tilde{\Phi} : \mathbb{R}^{k \times k} \rightarrow \mathbb{R}^{l \times l}$.*

Moreover, complete positivity of the map $\tilde{\Phi}$ is equivalent to positive semidefiniteness of the matrix $C = (C_{ij})_{i,j=1}^k = \sum_{i,j=1}^k (E_{ij} \otimes \tilde{\Phi}(E_{ij})) \in \mathcal{S}_{kl}$, where E_{ij} denotes the $k \times k$ -matrix with 1 in position (i, j) and zeros elsewhere.

A significant implication of Proposition 4.2 is the following. Given a linear subspace \mathcal{A} containing a positive definite matrix, a linear map $\Phi : \mathcal{A} \rightarrow \mathbb{R}^{l \times l}$ is completely positive if and only if at least one of all possible extensions of Φ to the whole matrix space is completely positive. The set of extensions is determined by linear equations, fixing some (but not all) of the entries in the matrix C . Testing the partially indeterminate matrix C for a positive semidefinite extension is a semidefinite feasibility problem (SDFP). Recall from the Preliminaries 2.1 that while the computational complexity of solving SDFPs is open, in practice it can be done efficiently by semidefinite programming. In Section 4.3 we apply this to containment of spectrahedra.

Surprisingly, positive maps on subspaces do not always have a positive extension to the full space; see, e.g., [39, Example 3.16]. And even if they do, characterizations of positive maps exist merely in low dimensions and in the setting of hermitian matrix algebras [42, 43]. The structure of positive maps on higher dimensional spaces is not completely understood [37, 38].

As we will see in this section, checking positivity of a map on subspaces is equivalent to checking containment for spectrahedra. We can thus apply our hierarchy for the containment question.

4.2. Equivalence of positive maps and containment. Given the linear pencils $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$, we call the linear pencil

$$(4.1) \quad \hat{A} = 1 \oplus A(x) = 1 \oplus A_0 + \sum_{p=1}^n x_p (0 \oplus A_p)$$

the *extended linear pencil* of $A(x)$, where \oplus denotes the direct sum of matrices. Define the corresponding linear subspaces

$$\begin{aligned}\mathcal{A} &= \text{span}(A_0, A_1, \dots, A_n) \subseteq \mathcal{S}_k, \\ \widehat{\mathcal{A}} &= \text{span}(1 \oplus A_0, 0 \oplus A_1, \dots, 0 \oplus A_n) \subseteq \mathcal{S}_{k+1}, \text{ and} \\ \mathcal{B} &= \text{span}(B_0, B_1, \dots, B_n) \subseteq \mathcal{S}_l.\end{aligned}$$

For linearly independent A_1, \dots, A_n , let $\widehat{\Phi}_{AB} : \widehat{\mathcal{A}} \rightarrow \mathcal{B}$ be the linear map defined by

$$\widehat{\Phi}_{AB}(1 \oplus A_0) = B_0 \quad \text{and} \quad \forall p \in \{1, \dots, n\} : \widehat{\Phi}_{AB}(0 \oplus A_p) = B_p.$$

Note that since every linear combination $0 = \lambda_0(1 \oplus A_0) + \sum_{p=1}^n \lambda_p(0 \oplus A_p)$ for real $\lambda_0, \dots, \lambda_n$ yields $\lambda_0 = 0$, it suffices to assume the linear independence of the coefficient matrices A_1, \dots, A_n to ensure that $\widehat{\Phi}_{AB}$ is well-defined. To obtain linear independence, the lineality space can be treated separately, as described in the Preliminaries 2.1. Note that the lineality space for the extended pencil is the same as for the actual pencil.

If additionally, A_0, A_1, \dots, A_n are linearly independent, we can retreat to the simpler map $\Phi_{AB} : \mathcal{A} \rightarrow \mathcal{B}$ defined by

$$\forall p \in \{0, \dots, n\} : \Phi_{AB} : A_p \mapsto B_p.$$

Assumption 4.3. Let A_0, \dots, A_n be linearly independent for statements concerning Φ_{AB} and let A_1, \dots, A_n be linearly independent for statements concerning $\widehat{\Phi}_{AB}$.

In [17, Theorem 3.5] the authors state the relationship between d -positive maps and the question of containment of (bounded) matricial positivity domains which for $d = 1$ contains the case of spectrahedra. The proof there is based on operator algebra. We give a more streamlined proof concerning positive maps and spectrahedra.

Proposition 4.4. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils.*

- (1) *If Φ_{AB} or $\widehat{\Phi}_{AB}$ is positive, then $S_A \subseteq S_B$.*
- (2) *If $S_A \neq \emptyset$, then $S_A \subseteq S_B$ implies $\widehat{\Phi}_{AB}$ is positive.*
- (3) *If $S_A \neq \emptyset$ and S_A is bounded, then $S_A \subseteq S_B$ implies Φ_{AB} is positive.*

Proof. To (1): Let Φ_{AB} be positive and let $x \in S_A$. Then $A(x) \succeq 0$. By the positivity of Φ_{AB} , we have $B(x) = \Phi_{AB}(A(x)) \succeq 0$, and thus $x \in S_B$. There is no difference in the proof if $\widehat{\Phi}_{AB}$ is positive.

To (2): First note that $A(x) \succeq 0$ if and only if the extended linear pencil $\widehat{A}(x)$ is positive semidefinite. Hence $S_A = S_{\widehat{A}}$. Set $\widehat{A}(x_0, x) := x_0(1 \oplus A_0) + \sum_{p=1}^n x_p(0 \oplus A_p)$ and let $x_0 \in \mathbb{R}$ with $\widehat{A}(x_0, x) \in \widehat{\mathcal{A}} \cap \mathcal{S}_{k+1}^+$. Then $x_0 \geq 0$.

Case $x_0 > 0$. Then $\widehat{A}(1, x/x_0) = \frac{1}{x_0} \widehat{A}(x_0, x) \succeq 0$. Thus, $\frac{x}{x_0} \in S_{\widehat{A}} = S_A \subseteq S_B$ and $B(x_0, x) = x_0 B(1, x/x_0) \succeq 0$. We get $\widehat{\Phi}_{AB}(\widehat{A}(x_0, x)) = B(x_0, x) \in \mathcal{B} \cap \mathcal{S}_l^+$.

Case $x_0 = 0$. By assumption, S_A is nonempty, i.e., there exists a point $\bar{x} \in S_A$. Then $A(0, x) \succeq 0$ together with the positive semidefiniteness of $A(1, \bar{x})$ (or, equivalently, $\widehat{A}(1, \bar{x})$) implies $\bar{x} + tx \in S_A \subseteq S_B$ for all $t \geq 0$. Thus x is a point of the recession cone of S_A which clearly is contained in the recession cone of S_B . Consequently, $\frac{1}{t} B(1, \bar{x}) + B(0, x) \succeq 0$ for

all $t > 0$. By closedness of the cone of positive semidefinite matrices, we get $B(0, x) \succeq 0$. Hence $\widehat{\Phi}_{AB}(\widehat{A}(x_0, x)) = \widehat{\Phi}_{AB}(\widehat{A}(0, x)) = B(0, x) \succeq 0$.

To (3): Let $S_A \subseteq S_B$ and $A(x_0, x) = x_0 A_0 + \sum_{p=1}^n x_p A_p \in \mathcal{A}$ be positive semidefinite.

Case $x_0 \leq 0$. Since S_A is nonempty, there exists $\bar{x} \in \mathbb{R}^n$ such that $A(1, \bar{x}) \succeq 0$, and hence

$$A(0, x + |x_0|\bar{x}) = A(0, x) + A(0, |x_0|\bar{x}) \succeq |x_0|A_0 + A(0, |x_0|\bar{x}) = |x_0| \cdot A(1, \bar{x}) \succeq 0.$$

For $A(0, x + |x_0|\bar{x}) \neq 0$, one has an improving ray of the spectrahedron S_A , in contradiction to the boundedness of S_A . For $A(0, x + |x_0|\bar{x}) = 0$, the linear independence of A_0, \dots, A_n implies $x + |x_0|\bar{x} = 0$. But then $x_0 A(1, \bar{x}) = A(x_0, x) \succeq 0$ together with $x_0 \leq 0$ and $A(1, \bar{x}) \succeq 0$ implies either $A(1, \bar{x}) = 0$, in contradiction to linear independence, or $(x_0, x) = 0$. Clearly, $\Phi_{AB}(0) = 0$.

Case $x_0 > 0$. Then $x/x_0 \in S_A \subseteq S_B$. Thus, $\Phi_{AB}(A(x_0, x)) = B(x_0, x) \succeq 0$. \square

The assumptions in parts (2) and (3) of Proposition 4.4 can not be omitted in general, as the next examples show.

Example 4.5. (1) Consider the two linear pencils

$$A(x) = \begin{bmatrix} -3 + x_1 + x_2 & 0 & 0 \\ 0 & -1 + x_1 & 0 \\ 0 & 0 & -1 + x_2 \end{bmatrix} \text{ and } B(x) = \begin{bmatrix} -1 + x_1 + x_2 & 0 & 0 \\ 0 & x_1 & 0 \\ 0 & 0 & x_2 \end{bmatrix}$$

defining unbounded, nonempty polyhedra in \mathbb{R}^2 . It is easy to see that the coefficient matrices are linearly independent and S_A does not contain the origin.

While S_A is contained in S_B , the linear map Φ_{AB} is not positive. Indeed, the homogeneous pencil $A(x_0, x)$ evaluated at the point $(x_0, x_1, x_2) = (-1, -1/2, -1/2)$ is positive definite while $B(x_0, x)$ is indefinite.

Therefore, the boundedness assumption in part (3) of Proposition 4.4 can not be omitted in general. Using the extended linear pencil $\widehat{A}(x) = 1 \oplus A(x)$ instead of $A(x)$, the resulting constraint $x_0 \geq 0$ yields the positivity of $\widehat{\Phi}_{AB}$. In fact, $\widehat{\Phi}_{AB}$ is completely positive, which can be checked by the SDFP (4.3) as introduced in the next subsection.

(2) Consider the two linear pencils

$$A(x) = \begin{bmatrix} x & 1 \\ 1 & 0 \end{bmatrix} \text{ and } B(x) = \begin{bmatrix} 1 & -x \\ -x & 1 \end{bmatrix}.$$

with linearly independent coefficient matrices. The corresponding spectrahedra are the empty set, $S_A = \emptyset$, and the interval $S_B = [-1, 1]$. Thus $S_A \subseteq S_B$. However, the linear map Φ_{AB} is not positive, since the homogeneous pencil $A(x_0, x)$ is positive semidefinite at $(x_0, x) = (0, 1)$ but $B(0, 1)$ is not. Note that this holds for the extended pencil as well. Thus nonemptiness of the inner spectrahedron can not be dropped. \square

Remark 4.6. If our setting were changed from the case of linear subspaces to the case of affine subspaces, with a natural adaption of the notion of positivity to affine maps, Proposition 4.4 had a slightly easier formulation and proof: Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$. Define the affine subspaces $\bar{\mathcal{A}} = \frac{1}{n}A_0 + \text{lin}(A_1, \dots, A_n)$ and $\bar{\mathcal{B}} = \frac{1}{n}B_0 + \text{lin}(B_1, \dots, B_n)$

for linearly independent A_1, \dots, A_n . Then $S_A \subseteq S_B$ if and only if the affine function $\bar{\Phi}_{AB} : \bar{\mathcal{A}} \rightarrow \bar{\mathcal{B}}$ defined by $\frac{1}{n}A_0 + A_i \mapsto \frac{1}{n}B_0 + B_i$ for $i = 1, \dots, n$ is positive.

Proof. First, let $\bar{\Phi}_{AB}$ be positive and let $x \in S_A$. Since $\bar{\Phi}_{AB}$ is positive, we have $B(x) = \bar{\Phi}_{AB}(A(x)) \succeq 0$, thus $x \in S_B$. Conversely, let $\frac{1}{n}A_0 + \sum_{p=1}^n x_p A_p \in \bar{\mathcal{A}} \cap \mathcal{S}_k^+$. Then $nx \in S_A \subseteq S_B$ and hence $\bar{\Phi}_{AB}(\frac{1}{n}A_0 + \sum_{p=1}^n x_p A_p) = \frac{1}{n}B_0 + \sum_{p=1}^n x_p B_p \succeq 0$. \square

4.3. Connection between complete positivity and containment criteria. Choosing a basis of \mathcal{A} , we get a representation of the operator map Φ_{AB} and by applying Proposition 4.4, we can use the hierarchy defined in the last section to test positivity of Φ_{AB} .

To keep the notation simple, we assume boundedness and nonemptiness of S_A , and only work with the map Φ_{AB} . All statements can be given in the general case using the map $\widehat{\Phi}_{AB}$. As seen before (see Section 4.1), every extension $\tilde{\Phi}_{AB}$ of the linear map Φ_{AB} to the full matrix spaces corresponds to a matrix $C = (\tilde{\Phi}_{AB}(E_{ij}))_{i,j=1}^k \in \mathcal{S}_{kl}$ perceiving C as a symmetric block matrix consisting of $k \times k$ blocks C_{ij} of size $l \times l$. Since A_0, \dots, A_n and B_0, \dots, B_n are generators of \mathcal{A} and \mathcal{B} , respectively, some entries of C are defined via $B_p = \sum_{i,j=1}^k a_{ij}^p C_{ij}$ for $p = 0, \dots, n$.

By Proposition 4.4, the polynomial optimization problem from Proposition 3.1 can be translated to the problem

$$(4.2) \quad \begin{aligned} & \inf \quad z^T B(x) z \\ & \text{s.t.} \quad B(x) = \sum_{i,j=1}^k (A(x))_{ij} C_{ij} \\ & \quad \quad G_A(x, z) \succeq 0. \end{aligned}$$

Moreover, (an extension of) Φ_{AB} is completely positive if and only if the matrix $C = (\tilde{\Phi}_{AB}(E_{ij}))_{i,j=1}^k \in \mathcal{S}_{kl}$ is positive semidefinite, i.e., if and only if the SDFP

$$(4.3) \quad C = (C_{ij})_{i,j=1}^k \succeq 0 \text{ and } B_p = \sum_{i,j=1}^k a_{ij}^p C_{ij} \text{ for } p = 0, \dots, n$$

has a solution. So checking if there exists a positive semidefinite $C \in \mathcal{S}_{kl}$, gives another sufficient criterion for the containment question. This is the method described in [17, 25].

Proposition 4.7. [25, Theorem 4.3] *If the SDFP (4.3) has a solution $C \succeq 0$, then $S_A \subseteq S_B$.*

In terms of the linear pencils, the previous proposition states that the pencil $B(x) = \sum_{i,j=1}^k (A(x))_{ij} C_{ij}$ is positive semidefinite if $A(x)$ and C are positive semidefinite, rendering the objective polynomial in (4.2) nonnegative on the set $S_A \times \mathbb{T}_{r,R}(0)$.

As we will see next, positive semidefiniteness of the matrix C is not only a sufficient condition for containment and thus for the nonnegativity of the polynomial optimization problem in Proposition 3.1, but also for its relaxations (3.2) and (3.4).

We show the following result:

Theorem 4.8. *Let $S_A \neq \emptyset$. Then for the properties*

- (1') $\widehat{\Phi}_{AB}$ is completely positive,
- (1) the SDFP (4.3) has a solution $C \succeq 0$,
- (2') $\lambda_{\text{sos}}(0) \geq 0$ (and thus $\lambda_{\text{sos}}(t) \geq 0$ for all $t \geq 0$),
- (2) $\mu_{\text{mom}}(2) \geq 0$ (and thus $\mu_{\text{mom}}(t) \geq 0$ for all $t \geq 2$),
- (3) $S_A \subseteq S_B$,
- (3') $\widehat{\Phi}_{AB}$ is positive,

we have the implications and equivalences

$$(1') \iff (1) \iff (2') \implies (2) \implies (3) \iff (3')$$

with the first implication an equivalence whenever \widehat{A} contains a positive definite matrix.

If, in addition, S_A is bounded, then $\widehat{\Phi}_{AB}$ in (1') and (3') can be replaced by Φ_{AB} .

Note that if the spectrahedron S_A is bounded, then Theorem 3.3 implies a partial converse of the implication (2) \implies (3). Namely, if $\emptyset \neq S_A \subseteq S_B$ and S_A is bounded, then $\mu_{\text{mom}}(t) \uparrow \mu \geq 0$ for $t \rightarrow \infty$.

Recalling Corollary 3.2 and Proposition 4.7, the remaining task is to prove (1) \implies (2) and (1) \iff (2'). The first is achieved in the following theorem. The proof of the second statement is straightforward. Indeed, by an easy computation one can check that for $t = 0$ the sos-matrix $S(x)$ is equal to (a permutation of) the matrix C coming from the SDFP (4.3) applied to the extended pencil.

Theorem 4.9. *If the SDFP (4.3) has a solution, then the infimum $\mu_{\text{mom}}(2)$ of the initial relaxation in (3.2) is nonnegative.*

Proof. Assume $C \succeq 0$ is a solution to the SDFP. Define the matrix C' via $(C'_{st})_{i,j} = (C_{ij})_{s,t}$, i.e., a $kl \times kl$ block matrix consisting of $l \times l$ blocks of size $k \times k$. Since it arises by permuting rows and columns of C simultaneously, C' is positive semidefinite as well.

Since (3.1) is feasible, the SDP (3.2) is feasible as well. For any (x, z) , the linearity of L_y implies for the objective in (3.2) (see also (4.2))

$$\begin{aligned} L_y(z^T B(x)z) &= L_y \left(z^T \sum_{i,j=1}^k (A(x))_{ij} C_{ij} z \right) = L_y \left(\sum_{i,j=1}^k \sum_{s,t=1}^l z_s z_t (A(x))_{ij} (C_{ij})_{s,t} \right) \\ &= \sum_{i,j=1}^k \sum_{s,t=1}^l L_y(z_s z_t (A(x))_{ij} (C_{ij})_{s,t}) = \mathbf{1}^T (L_y(z z^T \otimes A(x)) \odot C') \mathbf{1}, \end{aligned}$$

where \odot denotes the Hadamard product and $\mathbf{1} \in \mathbb{R}^{kl}$ is the all-one vector.

In the Hadamard product, the first matrix is positive semidefinite as a principal submatrix of $M_1(G_A y) = L_y(b_1(x, z) b_1(x, z)^T \otimes \text{diag}(A(x), g_r(z), g^R(z)))$ and $C' \succeq 0$ as stated above. By the Schur product theorem (see [22, Theorem 7.5.3]), the Hadamard product of the two matrices is positive semidefinite as well. Hence, $L_y(z^T B(x)z) \geq 0$ for any feasible y , and $\mu_{\text{mom}}(2) \geq 0$. \square

Remark 4.10. a) Theorem 4.9 can be stated for the polynomial optimization problem (3.1) itself. The proof is the same without the linearization operator L_y .

b) The reverse implication in Theorem 4.9 (and Theorem 4.8), i.e., (2) \implies (1), is not always true. Example 5.2 serves as a counterexample.

c) In terms of positive linear maps (see Section 4.1), Theorem 4.9 states that k -positivity is a sufficient condition for the initial relaxation step to certify containment. More generally, one can ask about the exact relationship between the exactness of the t -th relaxation step and $(k + 2 - t)$ -positivity of Φ_{AB} .

As seen in the proof of the last theorem, we can always represent the objective function of the optimization problem (3.2) in terms of a submatrix of $M_1(Ay)$ and the matrix C' (where the last one arises by permuting rows and columns of C simultaneously), $L_y(z^T B(x)z) = \mathbf{1}^T (L_y(zz^T \otimes A(x)) \odot C') \mathbf{1}$. In fact, this expression is just the trace or, equivalently, the scalar product of these two matrices, i.e.,

$$L_y(z^T B(x)z) = \text{tr} (L_y(zz^T \otimes A(x)) \cdot C') = \langle L_y(zz^T \otimes A(x)), C' \rangle.$$

Since $L_y(zz^T \otimes A(x))$ is a principal submatrix of $M_1(G_{Ay})$ which is constrained to be positive semidefinite, the first entry in the scalar product is positive semidefinite. Therefore, the question of whether the objective function is nonnegative on the feasible region reduces to the question of which conditions on the matrix C (or C') guarantee the nonnegativity of the scalar product on this set.

Using Theorem 4.9, we can extend the exactness results from [25] to the hierarchy (3.2), i.e., in some cases already the initial relaxation is not only a sufficient condition but also necessary for containment. More precisely, in these cases the equivalences (1) \iff (2') \iff (2) \iff (3) hold in Theorem 4.8. These results rely on the specific pencil representation of the given spectrahedra. Before stating the results, we have to agree on a consistent representation.

Every polyhedron $P = \{x \in \mathbb{R}^n : b + Ax \geq 0\}$ has a natural representation as a spectrahedron:

$$(4.4) \quad P = P_A = \left\{ x \in \mathbb{R}^n : A(x) = \begin{bmatrix} a_1(x) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & a_k(x) \end{bmatrix} \succeq 0 \right\},$$

where $a_i(x)$ abbreviates the i -th entry of the vector $b + Ax$. P_A contains the origin if and only if the inequalities can be scaled so that $b = \mathbf{1}_k$, where $\mathbf{1}_k$ denotes the all-ones vector in \mathbb{R}^k . Hence, in this case, $A(x)$ is monic, and it is called the *normal form* of the polyhedron P_A .

A centrally symmetric ellipsoid with axis-aligned semiaxes of lengths a_1, \dots, a_n can be written as the spectrahedron S_A of the monic linear pencil

$$(4.5) \quad A(x) = I_{n+1} + \sum_{p=1}^n \frac{x_p}{a_p} (E_{p,n+1} + E_{n+1,p}).$$

We call (4.5) the *normal form of the ellipsoid*. Specifically, for the case of all semiaxes having the same length $\nu := a_1 = \dots = a_n$, this gives the *normal form of a ball* with radius ν .

We are now ready to state the exactness results in Corollaries 4.11 and 4.12.

Corollary 4.11. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils. In the following cases, the initial relaxation step ($t = 2$) in (3.2) certifies containment of S_A in S_B .*

- (1) *if $A(x)$ and $B(x)$ are normal forms of ellipsoids (both centrally symmetric, axis-aligned semiaxes),*
- (2) *if $A(x)$ and $B(x)$ are normal forms of a ball and an \mathcal{H} -polyhedron, respectively,*
- (3) *if $B(x)$ is the normal form of a polytope,*
- (4) *if $\widehat{A}(x)$ (see (4.1)) is the extended form of a spectrahedron and $B(x)$ is the normal form of a polyhedron.*

Proof. Follows directly from [25, Theorem 4.8] and Theorem 4.9. □

Statements (2) to (4) in the previous corollary can also be deduced from the point of view of positive and completely positive maps introduced in Section 4.1. This follows from a result in [3, Proposition 1.2.2] stating that positive maps into commutative C^* -algebras are completely positive. The second exactness result states that the initial relaxation step can always certify containment of a scaled situation.

Corollary 4.12. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be monic linear pencils such that S_A is bounded. Then there exists $\nu > 0$ such that the initial relaxation step certifies $\nu S_A \subseteq S_B$, where $\nu S_A = \{x \in \mathbb{R}^n : A^\nu(x) := A(\frac{x}{\nu}) \succeq 0\}$ is the scaled spectrahedron.*

Proof. This follows from [25, Proposition 6.2] and Theorem 4.9. □

5. NUMERICAL EXPERIMENTS

While the complexity of the containment question for spectrahedra is co-NP-hard in general, the relaxation techniques introduced in this paper give a practical way of certifying containment. We implemented the hierarchy and applied it to several examples. The criterion performs well already for relaxation orders as low as $t = 2, 3$, as we will witness throughout this section.

We start by reviewing an example from [25] in Section 5.1, showing that the new hierarchical relaxation indeed outperforms the complete positivity relaxation. We then give an overview on the performance of the relaxation on some more examples.

In Section 5.2, we compare the results from the moment approach (3.2) to the alternative sum-of-squares approach (3.4). To assess the performance of both algorithms, we compare results as well as runtimes of the algorithms on randomly generated pencils of varying sizes.

We use the example of computing the symmetric circumradius of a spectrahedron to show how the relaxation can be simplified in the case when the outer spectrahedron can be described as the positivity region of a single polynomial. This is discussed in Section 5.3.

For our computations, we modeled the hierarchy using high-level YALMIP [30, 31] code. We used MOSEK 7 [2] as external solver for the optimization problems defined in YALMIP. The MATLAB version used was R2011b, running on a desktop computer with Intel Core i3-2100 @ 3.10 GHz and 4 GB of RAM.

Throughout this section, we use the following notation. As before, integer n stands for the number of variables in the pencils, k and l for the size of the pencil $A(x)$ and

ν	SDFP (4.3)	$\mu_{\text{mom}}(2)$	sec	$\mu_{\text{mom}}(3)$	sec
0.7	feasible	0.0101	0.11	0.300	0.17
0.707	feasible	0.000151	0.1	0.293	0.16
$1/\sqrt{2}$	feasible	$7.29 \cdot 10^{-11}$	0.09	0.293	0.16
0.708	infeasible	-0.000632	0.1	0.292	0.16
0.8	infeasible	-0.0657	0.09	0.200	0.16
1	infeasible	-0.207	0.1	$9.78 \cdot 10^{-09}$	0.19
1.1	infeasible	-0.278	0.1	-0.100	0.16

TABLE 1. Disk νS_A in disk S_B for two different representations and various radii ν of the inner disk as described in Example 5.1.

$B(x)$, respectively. For monic pencils, we examine ν -scaled spectrahedra νS_A as defined in Corollary 4.12. We denote the (numerical) optimal value of the moment relaxation (3.2) of order t by $\mu_{\text{mom}}(t)$, the (numerical) optimal value of the alternative relaxation (3.4) of order t by $\lambda_{\text{sos}}(t)$. In the tables, “sec“ states the time in seconds for setting up the problem in YALMIP and solving it in MOSEK.

If not stated otherwise, the inner radius is set to $r = 1$ and outer radius to $R = 2$ in relaxation (3.2).

5.1. Numerical computations. We review the example of containment of two disks from [25]. The complete positivity criterion from that work certifies the containment only if the disk on the inside is scaled small enough. Theorem 4.9 shows that any containment certified by the complete positivity criterion is certified by the hierarchical relaxation. In the following example we go one step further, showing that the latter performs strictly better than the feasibility criterion already in small relaxation orders.

Example 5.1. Consider the monic linear pencils $A^\nu(x) = I_3 + x_1 \frac{1}{\nu}(E_{1,3} + E_{3,1}) + x_2 \frac{1}{\nu}(E_{2,3} + E_{3,2}) \in \mathcal{S}_3[x]$ with parameter $\nu > 0$ and $B(x) = I_2 + x_1(E_{1,1} - E_{2,2}) + x_2(E_{1,2} + E_{2,1}) \in \mathcal{S}_2[x]$. The spectrahedra defined by the pencils are the disk of radius $\nu > 0$ centered at the origin, $\nu S_A = \mathbb{B}_\nu(0)$, and the unit disk $S_B = \mathbb{B}_1(0)$, respectively. Clearly, $\nu S_A \subseteq S_B$ if and only if $0 < \nu \leq 1$. In particular, for $\nu = 1$, both pencils define the unit disk $\mathbb{B}_1(0) = S_A = S_B$.

In [25, Section 6.1] it is shown that the complete positivity criterion for the containment problem $\nu S_A \subseteq S_B$ is satisfied if $0 < \nu \leq \frac{1}{2}\sqrt{2}$. Remarkably, the performance of relaxation (3.2) depends on the choice of the parameters r and R . Table 1 contrasts the results of the moment relaxation with parameters $r = 1, R = 2$ with the results of the complete positivity criterion for the problem $\nu S_A \subseteq S_B$. Our numerical computations shows that the semidefinite relaxation of order $t = 2$ certifies the same cases as the complete positivity criterion. For $t = 3$ we have exactness of the criterion.

When choosing $r = R = 1$, the semidefinite relaxation (3.2) is exact already for relaxation order $t = 2$ and returns the same optimal values as for relaxation order $t = 3$. This choice of parameters however leads to numerical problems in the solver occasionally. Furthermore the example of the two disks is the only one we have found, where results for

size			objective value		sec	
n	k	l	$\mu_{\text{mom}}(2)$	$\lambda_{\text{sos}}(0)$	$\mu_{\text{mom}}(2)$	$\lambda_{\text{sos}}(0)$
3	4	3	0.293	0.293	0.12	0.81
6	7	4	0.134	0.134	1.46	0.77
10	11	5	0.106	$-3.972 \cdot 10^{-8}$	28.51	3.61
15	16	6	0.087	-0.118	588.57	65.47

TABLE 2. Computational test of containment of ball in ellipptope as described in Example 5.2.

orders $t = 2$ and $t = 3$ differ if r and R are chosen distinct. In all other examples, results seem to be exact already for $t = 2$. Therefore we advise to use $r = 1$ and $R = 2$ in general applications. \square

In the next example, we examine the containment of a ball in an ellipptope. The ellipptope is a nice example of a spectrahedron that is described by a pencil consisting of very sparse matrices. While the pencil is of small size, it is occupied by a large number of variables.

Example 5.2. For this example, the pencil description of the ball is as in (4.5). The *ellipptope* (5.2) can be described as the positivity domain of a symmetric pencil with ones on the diagonal and distinct variables in the remaining positions; see [6, Section 2.1.3].

As exhibited in Table 2, the ball of radius $\frac{1}{2}$ in dimensions $n = 3, 6, 10$ and 15 is contained in the ellipptope of the respective dimension. The computational time grows in the number of variables, but even dimensions as high as 15 are in the scope of desktop computers if the size l of the pencil $B(x)$ is moderate.

Interestingly, while the moment relaxation is slower than the sum-of-squares approach in this example (for $t = 0$ and $t = 2$, respectively), the latter approach fails to be exact in dimension $n = 10, 15$. When trying to compute the next relaxation step $\lambda_{\text{sos}}(1)$ for $(n, k, l) = (10, 11, 5)$, we stopped the computation after about 15 hours. Note that the SDFP (4.3) is solvable for $(n, k, l) = (10, 11, 5)$ but not solvable for $(n, k, l) = (15, 16, 6)$. Thus, for $(n, k, l) = (15, 16, 6)$, this example serves as a counterexample for the reverse statement of Theorem 4.9 (or, equivalently, for the implication (2) \implies (1) in Theorem 4.8). \square

Example 5.3. Consider the linear map

$$\Phi : \mathcal{S}_3 \rightarrow \mathcal{S}_3, A \mapsto 2 \begin{bmatrix} A_{11} + A_{22} & & \\ & A_{22} + A_{33} & \\ & & A_{33} + A_{11} \end{bmatrix} - A.$$

Due to Choi [8], the map Φ is (1- and 2-)positive but not completely positive. Indeed, the SDFP (4.3) is not feasible. Using hierarchy (3.2) (with $r = R = 1$), the initial relaxation step is also not feasible but for $t = 3$ the relaxation yields a small positive value implying positivity of Φ . \square

no.	size			objective value				sec			
	n	k	l	$\mu_{\text{mom}}(2)$	$\mu_{\text{mom}}(3)$	$\lambda_{\text{sos}}(0)$	$\lambda_{\text{sos}}(1)$	$\mu_{\text{mom}}(2)$	$\mu_{\text{mom}}(3)$	$\lambda_{\text{sos}}(0)$	$\lambda_{\text{sos}}(1)$
1	2	4	4	0.330	0.330	0.330	0.330	0.26	2.49	0.29	2.04
2	2	6	4	1.459	1.459	1.459	1.459	0.16	2.95	0.34	9.98
3	2	4	6	-2.009	-2.009	-2.009	-2.009	0.38	31.03	0.42	10.61
4	2	6	6	-0.209	-0.209	-0.209	-0.209	0.36	31.53	0.72	76.23
5	3	4	4	0.156	0.156	0.156	0.156	0.20	6.35	0.30	3.83
6	3	6	4	0.332	0.332	0.332	0.332	0.22	8.86	0.34	24.52
7	3	4	6	-6.918	-6.906	-6.918	-6.918	0.82	117.3	0.45	28.3
8	3	6	6	0.028	0.028	0.028	0.028	0.66	84.71	0.71	207.84
9	4	4	4	-3.164	-3.164	-3.164	-3.164	1.33	32.64	0.97	10.19
10	4	6	4	0.593	0.593	0.593	0.593	0.32	27.88	0.35	66.39
11	4	4	6	-0.938	-0.938	-0.938	-0.938	1.21	326	0.45	64.41
12	4	6	6	-0.251	-0.251	-0.251	-0.251	1.43	317.08	0.81	567.07

TABLE 3. Computational test of containment of randomly generated spectrahedra as described in Example 5.4.

5.2. Randomly Generated Spectrahedra. We applied both hierarchical criteria, the moment hierarchy (3.2) and the alternative sum-of-squares approach (3.4) to several instances of linear pencils with random entries.

For the experiments in this section, we generate coefficient matrices A_1, \dots, A_n by assigning random numbers to the off-diagonal entries of the matrices. Numbers are drawn from a uniform distribution on $[-1, 1]$. The generated matrices are sparse in the sense that roughly 35% of the off-diagonal entries are nonzero. The matrix for the constant term, A_0 , is generated in the same way, but features ones on the diagonal. This choice leads to bounded spectrahedra in most cases, namely when the matrices A_0, \dots, A_k are linearly independent. Unbounded spectrahedra and spectrahedra without interior are discarded.

The pencil of the second spectrahedron S_B is generated in the same way, except that the diagonal entries of B_0 are chosen larger. This has the effect that the corresponding spectrahedra are scaled and the containment $S_A \subseteq S_B$ is more likely to happen.

Example 5.4. We apply the hierarchies to a range of problems with varying dimensions and pencil sizes as reported in Table 3. To illustrate the approach, we provide the pencils for experiment no. 1 below.

$$A(x) = \begin{bmatrix} 1 & 0.2528x_1 + 0.3441x_2 & 0 & 0 \\ 0.2528x_1 + 0.3441x_2 & 1 & 0 & -0.1314x_1 \\ 0 & 0 & 1 & 0.7969x_2 \\ 0 & -0.1314x_1 & 0.7969x_2 & 1 \end{bmatrix}$$

$$B(x) = \begin{bmatrix} 2 & 0.8454 & 0 & 0 \\ 0.8454 & 2 & -0.2489x_1 - 0.4063x_2 & 0 \\ 0 & -0.2489x_1 - 0.4063x_2 & 2 & 0.3562x_1 \\ 0 & 0 & 0.3562x_1 & 2 \end{bmatrix}$$

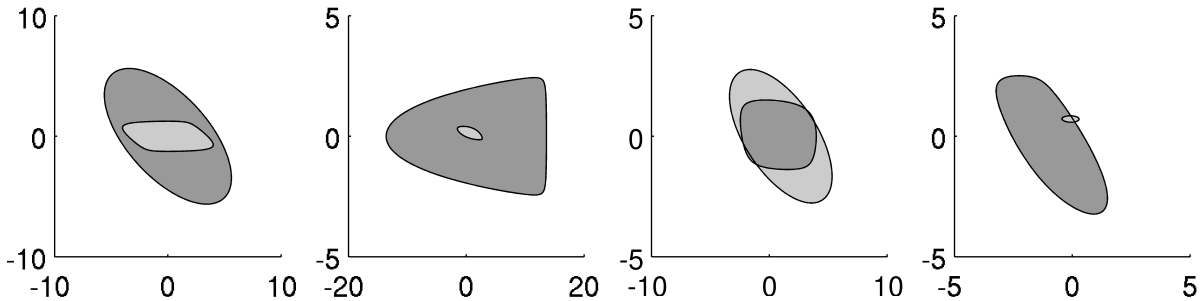


FIGURE 1. Spectrahedra of experiments no. 1–4 from Table 3. S_A : light grey, S_B : dark grey.

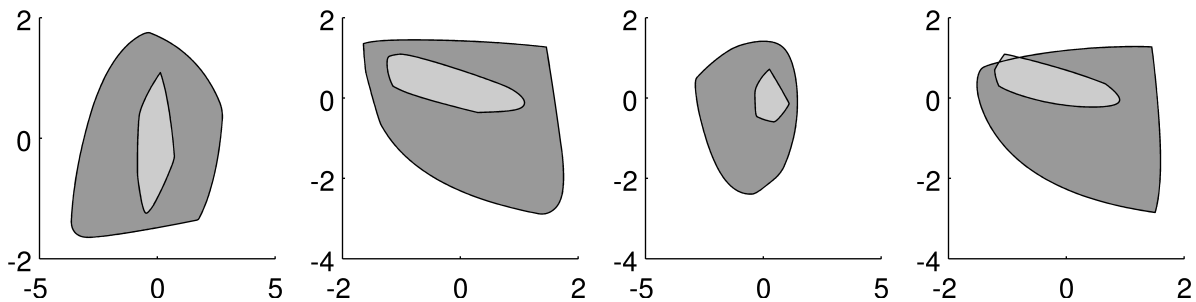


FIGURE 2. Projections of the 4-dimensional spectrahedron no. 12 from Table 3. S_A : light grey, S_B : dark grey. Projections to planes spanned by (x_1, x_2) , (x_2, x_3) , (x_3, x_4) and $(0.3x_1 + x_2, x_3)$.

For this experiment with randomly generated matrices, the truth value of the containment question is unknown a priori. In the case of a positive objective value, our criterion yields a certificate for the containment. For negative objective values, we inspected plots of the spectrahedra to check appropriateness of the criterion. Plots of the spectrahedra from the two-dimensional experiments no. 1–4 are shown in Figure 1.

In cases of higher dimension ($n > 3$), we examined projections of the spectrahedra. See Figure 2 for projections of the spectrahedra from experiment no. 12 to different planes. The small negative objective value reported in Table 3 suggests that there is only a small overlap of S_A over the boundary of S_B . Indeed, the projections to the coordinate planes suggest that S_A is contained in S_B . But when projecting to the plane spanned by $0.3x_1 + x_2$ and x_3 , we see that the spectrahedra are not contained.

In all cases we examined, the results from the criterion correspond with the expectations we had from inspecting the plots. Remarkably, for the randomly generated spectrahedra, the results of the relaxations match closely across different relaxation orders and across the two approaches discussed. This suggests that the criteria perform well in generic cases.

Concerning running times, both approaches are comparable. As expected, running times increase quickly with growing dimension n and with an increase in the dimension l of the pencil $B(x)$. This is due to the fact, that the number of linearization variables grows when these parameters are increased, as discussed in Section 3.3.

Remarkably, the number of linearization variables in the moment approach does not depend on the size k of the pencil $A(x)$. While the size of the matrix in the resulting semidefinite program depends on k , the number of variables plays a more important role. Indeed, the running times for the moment approach are not influenced much by an increase in the size of the pencil $A(x)$. As witnessed in Table 3, the running times for the moment approach may even decrease slightly for larger k . Thus for problems with relatively large k , the moment approach should be used, since it seems to be superior to the alternative approach in this case. \square

From the examples discussed here and in Section 5.1, it is not clear whether one of the approaches (3.2) and (3.4) is globally better than the other. While the moment approach (3.2) outperforms the sos-approach in Example 5.2 for $(n, k, l) = (10, 11, 5)$ and, e.g., in the experiments no. 8, 12, the sos-approach (3.4) is significantly faster in the experiments no. 7, 11.

5.3. Geometric radii. Let $A(x) \in \mathcal{S}_k[x]$ be a linear pencil and denote by $B(\nu, p; x)$ the normal form (4.5) of the ball $\mathbb{B}_\nu(p) \subseteq \mathbb{R}^n$ with radius $\nu > 0$ centered at some point $p \in \mathbb{R}^n$. Consider the problem of determining whether the spectrahedron S_A is contained in $\mathbb{B}_\nu(p)$.

As seen in Section 3.1, S_A is contained in $\mathbb{B}_\nu(p)$ if and only if $B(\nu, p; x)$ is positive semidefinite on S_A . Since $B(\nu, p; x) \succeq 0$ is equivalent to the nonnegativity of the polynomial $\nu^2 - (x - p)^T(x - p)$, the polynomial optimization problem (3.1) can be simplified to

$$\begin{aligned} \min \quad & \nu^2 - (x - p)^T(x - p) \\ \text{s.t.} \quad & A(x) \succeq 0 \end{aligned}$$

Hence, $S_A \subseteq \mathbb{B}_\nu(p)$ for fixed p with minimal possible $\nu > 0$ if and only if

$$(5.1) \quad \begin{aligned} \nu^2 = \max \quad & (x - p)^T(x - p) \\ \text{s.t.} \quad & A(x) \succeq 0. \end{aligned}$$

If the spectrahedron S_A is centrally symmetric, i.e., $x \in S_A$ implies $-x \in S_A$, then by choosing the origin $p = 0$ as the center of the ball this polynomial optimization problem computes the circumradius of S_A . In general, computing the circumradius is a min-max-problem, as one has to compute the minimum of the above maximum over all $p \in \mathbb{R}^n$.

This also gives a certificate for boundedness of S_A . Indeed, S_A is bounded if and only if the program (5.1) has a finite value.

As in Section 3.2, using a moment relaxation, we can derive a semidefinite hierarchy for the containment problem of a spectrahedron in the ball $\mathbb{B}_\nu(p)$. If the unique circumcenter of S_A is a priori known, then the hierarchy yields upper bounds for the circumradius of the spectrahedron. Since the objective polynomial involves only monomials of degree 2, the relaxation performs very well; see Table 4 for exemplary results on the elliptope. For this case, the stated values of the initial relaxation are indeed optimal.

Lemma 5.5. *For the elliptope in dimension $n = k(k - 1)/2$ for some integer $k > 2$ the circumradius equals \sqrt{n} .*

Proof. Since the origin is the only point of the elliptope which is invariant under the switching symmetry [29], it is the center point of the smallest enclosing ball.

S_A	n	$\nu^2(2)$	sec
elliptope	3	3.00	0.51
	6	6.00	0.51
	10	10.00	1.02
	15	15.00	16.43

TABLE 4. Circumradius of the elliptope. Here $\nu^2(2)$ denotes the numerical optimal value of the moment relaxation of order $t = 2$.

Let $x \in S_A$, where S_A is the elliptope given by the linear pencil

$$(5.2) \quad A(x) = I_n + \sum_{1 \leq i < j \leq k} x_{ij}(E_{i,j} + E_{j,i}).$$

Consider the 2×2 principal minors of $A(x)$. Then $1 - x_i^2 \geq 0$ for all $i = 1, \dots, n$. Summing up yields $n - \sum_{i=1}^n x_i^2 \geq 0$, and hence $x \in \mathbb{B}_{\sqrt{n}}(0)$. On the other hand, since every principal submatrix of $A(\mathbf{1})$ is an all-one-matrix, and hence the determinant (of every principal minor) vanishes, we get $\mathbf{1} \in \partial S_A$. (Note that the linear pencil is reduced in the sense of Proposition 2.1). Thus $\mathbf{1} \in \partial \mathbb{B}_{\sqrt{n}}(0) \cap \partial S_A$, implying the claim. \square

Note that the hierarchical approach provides an improvement over the solitary relaxation (“matricial radius”) studied by Helton, Klep, and McCullough [17].

Remark 5.6. As seen by a standard example in semidefinite programming (see, e.g., [1, 11]), there exists a spectrahedron whose elements have a coordinate of double-exponential size in the number of variables and hence double-exponential distance (to the origin) in the number of variables. Therefore we cannot in general expect to attain a certificate for the boundedness of the spectrahedron that is polynomial in the input size.

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