CONTAINMENT PROBLEMS FOR POLYTOPES AND SPECTRAHEDRA

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ABSTRACT. We study the computational question whether a given polytope or spectrahedron S_A (as given by the positive semidefiniteness region of a linear matrix pencil $A(x)$) is contained in another one S_B.

First we classify the computational complexity, extending results on the polytope/polytope-case by Gritzmann and Klee to the polytope/spectrahedron-case. For various restricted containment problems, NP-hardness is shown.

We then study in detail semidefinite conditions to certify containment, building upon work by Ben-Tal, Nemirovski and Helton, Klep, McCullough. In particular, we discuss variations of a sufficient semidefinite condition to certify containment of a spectrahedron in a spectrahedron. It is shown that these sufficient conditions even provide exact semidefinite characterizations for containment in several important cases, including containment of a spectrahedron in a polyhedron. Moreover, in the case of bounded S_A the criteria will always succeed in certifying containment of some scaled spectrahedron νS_A in S_B.

1. INTRODUCTION

Denote by $\mathcal{S}_k$ the set of all real symmetric $k \times k$-matrices and by $\mathcal{S}_k[x]$ the set of symmetric $k \times k$-matrices with polynomial entries in $x = (x_1, \ldots, x_n)$. For $A_0, \ldots, A_n \in \mathcal{S}_k$, let $A(x)$ denote the *linear (matrix) pencil* $A(x) = A_0 + x_1 A_1 + \cdots + x_n A_n \in \mathcal{S}_k[x]$. Then the set

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

is called a *spectrahedron*, where $A(x) \succeq 0$ denotes positive semidefiniteness of the matrix $A(x)$.

Spectrahedra arise as feasible sets of semidefinite programming (see [8, 25]). In the last years, there has been strong interest in understanding the geometry of spectrahedra (see, e.g., [1, 10, 18]), particularly driven by their intrinsic relevance in polynomial optimization [4, 11] and convex algebraic geometry [19, 20]. Spectrahedra naturally generalize the class of polyhedra, see [3, 27] for particular connections between these two classes.

In this paper, we study containment problems for polyhedra and spectrahedra. Since polyhedra are special cases of spectrahedra, we can use the following general setup: Given two linear pencils $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$, is $S_A \subseteq S_B$?

For polytopes (i.e., bounded polyhedra), the computational geometry and computational complexity of containment problems have been studied in detail. See in particular the classifications by Gritzmann and Klee [12, 13, 14]. Notably, it is well-known that the computational complexity of deciding containment problems strongly depends on the type

of the input. For instance, if both polytopes are given by their vertices ($\mathcal{V}$-polytopes), or both polytopes are given as an intersection of halfspaces ($\mathcal{H}$-polytopes), containment can be decided in polynomial time, while it is co-NP-hard to decide whether an $\mathcal{H}$-polytope is contained in a $\mathcal{V}$-polytope (see [7, 14]).

For spectrahedra, much less is known. Ben-Tal and Nemirovski studied the matrix cube problem [2], which corresponds to the containment problem where S_A is a cube. In a much more general setting, Helton, Klep, and McCullough [16] studied containment problems of matricial positivity domains (which live in a union of spaces of different dimensions). As a byproduct, they also derive some implications for containment of spectrahedra.

In the current paper, we study containment problems of polytopes, polyhedra and spectrahedra from a computational viewpoint. In Section 3, we extend existing complexity classifications for the polyhedral situation to the situation where polytopes and spectrahedra are involved. In particular, the containment question of a $\mathcal{V}$-polytope in a spectrahedron can be decided in polynomial time, and the question whether a spectrahedron is contained in an $\mathcal{H}$-polytope can be formulated by the complement of semidefinite feasibility problems (involving also strict inequalities). Roughly speaking, the other cases are co-NP-hard. This includes the containment problem of an $\mathcal{H}$-polytope in a spectrahedron, already when the spectrahedron is a ball. The complete classification is stated in Theorems 3.2–3.4.

To overcome the situation that the general containment problem for spectrahedra is co-NP-hard, relaxation techniques are of particular interest. Our point of departure in Section 4 is the relaxation from [16] which provides a distinguished sufficient criterion for containment of a spectrahedron S_A in a spectrahedron S_B (see (4.2)). We provide an elementary derivation of this semidefinite relaxation (as opposed to the operator-theoretic techniques used there) and study the quality of the criterion. This leads to a new and systematic access to studying containment problems of polyhedra and spectrahedra and provides several new (and partially unexpected) results.

In particular, we obtain the following new results:

1. We discuss variations of containment criterion (4.2), which lead to improved numerical results, see Theorem 4.3, Corollaries 4.6 and 4.7 and Section 6.1.

2. We exhibit several cases when the criteria are exact (see Theorem 4.8). For some of the cases we can provide elementary proofs. The main case in Theorem 4.8 states that the sufficient criteria for the containment of spectrahedra in polyhedra (in normal form) are *exact* characterizations. The proof of the statements is given in Section 5, by developing various properties of the containment criteria (transitivity, block diagonalization) and combining them with duality theory of semidefinite programming. The exactness of the spectrahedron-polyhedron-case is particularly surprising, since a priori the criteria depend on the linear pencil representation of the spectrahedron.

3. In Section 6.1, we extend the results from [16] on cases, where the criteria are not exact. For a counterexample in [16] we exhibit the phenomenon that the containment criteria will at least succeed in certifying that a scaled version of the spectrahedron S_A is contained in S_B.

4. In Proposition 6.2, we show that in the case of bounded S_A there *always* exists a scaling factor $\nu > 0$ such that for the scaled spectrahedron pair $(\nu S_A, S_B)$ the criteria (4.2) and (4.3) hold.

We will close the paper by explaining some implications of the scaling result on the optimization version of containment problems (as also relevant for the computation of geometric radii of convex bodies, e.g., in [12, 13]).

2. PRELIMINARIES

Throughout the paper we work in n-dimensional Euclidean space $\mathbb{R}^n$, and $\|\cdot\|$ denotes the Euclidean norm.

Matrices and block matrices. For a matrix A, the (i, j)-th entry of A is labeled by a_{ij} as usual. For a block matrix B, we label the (i, j)-th block by B_{ij} and the (s, t)-th entry of B_{ij} by $(B_{ij})_{st}$.

A square matrix with 1 in the entry (i, j) and zeros otherwise is denoted by E_{ij}. The $n \times n$ identity matrix is denoted by I_n.

The *Kronecker product* $A \otimes B$ of square matrices A of size $k \times k$ and B of size $l \times l$ is the $kl \times kl$ matrix

$$(2.1) \qquad A \otimes B = \begin{bmatrix} a_{11} B & \dots & a_{1k} B \\ \vdots & \ddots & \vdots \\ a_{k1} B & \dots & a_{kk} B \end{bmatrix}$$

(see, e.g., [6, 21]). It is well-known (see, e.g., [21, Cor. 4.2.13]) that the Kronecker product of two positive semidefinite matrices is again positive semidefinite.

Polyhedra and polytopes. A *polyhedron* is the intersection of finitely many halfspaces. A bounded polyhedron or, equivalently, the convex hull of finitely many points in $\mathbb{R}^n$ is called *polytope*.

For algorithmic questions in n-dimensional space it is crucial whether a polytope is given in the first way ($\mathcal{H}$-*polytope*) or in the second way ($\mathcal{V}$-*polytope*). Our model of computation is the binary Turing machine: polytopes are presented by certain rational numbers, and the size of the input is defined as the length of the binary encoding of the input data (see, e.g., [12]). A $\mathcal{V}$-polytope P is given by a tuple $(n; m; v^{(1)}, \dots, v^{(m)})$ with $n, m \in \mathbb{N}$, and $v^{(1)}, \dots, v^{(m)} \in \mathbb{Q}^n$ such that $P = \mathrm{conv}\{v^{(1)}, \dots, v^{(m)}\}$. An $\mathcal{H}$-polytope P is given by a tuple $(n; m; A; b)$ with $n, m \in \mathbb{N}$, a rational $m \times n$-matrix A, and $b \in \mathbb{Q}^m$ such that $P = \{x \in \mathbb{R}^n : b + Ax \geq 0\}$ is bounded. If the i-th row $(b + Ax)_i \geq 0$ defines a facet of P, then the i-th row of A is an *inner* normal vector of this facet.

For fixed dimension, $\mathcal{H}$- and $\mathcal{V}$-presentations of a rational polytope can be converted into each other in polynomial time. In general dimension (i.e., if the dimension is not fixed but part of the input) the size of one presentation can be exponential in the size of the other [24].

Spectrahedra. Given a linear pencil

$$(2.2) \qquad A(x) \; = \; A_0 + \sum_{p=1}^{n} x_p A_p \in \mathcal{S}_k[x] \quad \text{with } A_p = (a_{ij}^p), \quad 0 \le p \le n,$$

the spectrahedron $S_A = \{x \in \mathbb{R}^n \,:\, A(x) \succeq 0\}$ contains the origin in its interior if and only if there is another linear pencil $A'(x)$ with the same positivity domain such that $A_0' = I$, see [8, 20]. In particular, then S_A is full-dimensional. To simplify notation, we sometimes assume that $A(x)$ is a *monic* linear pencil, i.e. $A_0 = I_k$. As a shorthand we use $A \succeq B$ to state that $A - B$ is positive semidefinite.

Note that every polyhedron $P = \{x \in \mathbb{R}^n \,:\, b + Ax \ge 0\}$ has a natural representation as a spectrahedron:

$$(2.3) \qquad P = P_A = \left\{ x \in \mathbb{R}^n \,:\, A(x) = \begin{bmatrix} a_1(x) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & a_k(x) \end{bmatrix} \succeq 0 \right\},$$

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 $b = \mathbb{1}_k$, where $\mathbb{1}_k$ 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 semi-axes of lengths $a_1, \dots, a_n$ can be written as the spectrahedron S_A of the monic linear pencil

$$(2.4) \qquad A(x) \; = \; I_{n+1} + \sum_{p=1}^{n} \frac{x_p}{a_p}(E_{p,n+1} + E_{n+1,p}).$$

We call (2.4) the *normal form of the ellipsoid*. Specifically, for the case of equal semi-axis lengths $r := a_1 = \cdots = a_n$ this gives the *normal form of a ball* with radius r.

For algorithmic questions, a linear pencil is given by a tuple $(n; k; A_0, \dots, A_n)$ with $n, k \in \mathbb{N}$ and $A_0, \dots, A_n$ rational symmetric matrices.

3. Complexity of containment problems for spectrahedra

In this section, we classify the complexity of several natural containment problems for spectrahedra. For polytopes the computational complexity of containment problems strongly depends on the type of input representations. For $\mathcal{V}$- and $\mathcal{H}$-presented polytopes, the following result is well-known (see [7, 14]).

Proposition 3.1. *Deciding whether a polytope P is contained in a polytope Q can be done in polynomial time for the following cases:*

(1) *Both P and Q are $\mathcal{H}$-polytopes,*
(2) *both P and Q are $\mathcal{V}$-polytopes, or*
(3) *P is a $\mathcal{V}$-polytope while Q is an $\mathcal{H}$-polytope.*

However, deciding whether an $\mathcal{H}$-polytope is contained in a $\mathcal{V}$-polytope is co-NP-complete. This hardness persists if P is restricted to be a standard cube and Q is restricted to be the affine image of a cross polytope.

In the next statements we extend this classification to containment problems involving polytopes and spectrahedra. See Table 1 for a summary. Theorems 3.2 and 3.3 give the positive results.

	$\mathcal{H}$	$\mathcal{V}$	$\mathcal{S}$
$\mathcal{H}$	P	co-NP-complete	co-NP-hard
$\mathcal{V}$	P	P	P
$\mathcal{S}$	"SDP"	co-NP-hard	co-NP-hard

TABLE 1. Computational complexity of containment problems, where the rows refer to the inner set and the columns to the outer set and $\mathcal{S}$ abbreviates spectrahedron.

Theorem 3.2. *Deciding whether a $\mathcal{V}$-polytope is contained in a spectrahedron can be done in polynomial time.*

Proof. Given a $\mathcal{V}$-presentation $P = \mathrm{conv}\{v^{(1)}, \ldots, v^{(m)}\}$ and a linear matrix pencil $A(x)$, we have $P \subseteq S_A$ if and only if all the points $v^{(i)}$ are contained in S_A. Thus, the containment problem is reduced to m tests whether a certain rational matrix is positive semidefinite. This can be decided in polynomial time, as one can compute, for a rational, symmetric matrix A, a decomposition $A = UDU^T$ with a diagonal matrix D in polynomial time (see, e.g., [9]). $\square$

Containment questions for spectrahedra are connected to feasibility questions of semidefinite programs in a natural way. A Semidefinite Feasibility Problem (SDFP) is defined as the following decision problem (see, e.g., [26]): Given a linear pencil defined by a tuple $(n; k; A_0, \ldots, A_n)$ with $n, k \in \mathbb{N}$ and $A_0, \ldots, A_n$ rational symmetric matrices. Are there real numbers $x_1, \ldots, x_n$ such that $A(x) = A_0 + \sum_{p=1}^{n} x_p A_p \succeq 0$, or equivalently, is the spectrahedron S_A non-empty?

Although semidefinite programs can be approximated up to an additive error of ε in polynomial time, the question "SDFP $\in$ P?" is one of the major open complexity questions in semidefinite programming (see [6, 26]). Consequently, the following statement on containment of a spectrahedron in an $\mathcal{H}$-polytope does not give a complete answer concerning polynomial solvability of these containment questions in the Turing machine model. If the additional inequalities were non-strict, then we had to decide a finite set of problems from the complement of the class SDFP.

Theorem 3.3. *The problem of deciding whether a spectrahedron is contained in an $\mathcal{H}$-polytope can be formulated by the complement of semidefinite feasibility problems (involving also strict inequalities), whose sizes are polynomial in the description size of the input data.*

Proof. Let $A(x)$ be a linear matrix pencil and $P = \{x \in \mathbb{R}^n : b + Bx \geq 0\}$ with $B \in \mathbb{Q}^{m \times n}$ be an $\mathcal{H}$-polytope. For each $i \in \{1, \ldots, m\}$ incorporate the linear condition $b_i + \sum_{j=1}^{n} b_{ij} x_j < 0$ into the linear pencil $A(x)$. If one of the resulting m ("semi-open") spectrahedra is nonempty then $S_A \not\subseteq P$. $\square$

The positive results in Theorems 3.2 and 3.3 are contrasted by the following hardness results.

Theorem 3.4.
  (1) *Deciding whether a spectrahedron is contained in a $\mathcal{V}$-polytope is co-NP-hard.*
  (2) *Deciding whether an $\mathcal{H}$-polytope or a spectrahedron is contained in a spectrahedron is co-NP-hard. This hardness statement persists if the $\mathcal{H}$-polytope is a standard cube or if the outer spectrahedron is a ball.*

Proof. Deciding whether a spectrahedron S_A is contained in a $\mathcal{V}$-polytope is co-NP-hard since already deciding whether an $\mathcal{H}$-polytope is contained in a $\mathcal{V}$-polytope is co-NP-hard by Proposition 3.1.

Concerning the second statement, co-NP-hardness of containment of $\mathcal{H}$-polytopes in spectrahedra follows from Ben-Tal and Nemirovski [2, Proposition 4.1], who use a reduction from the maximization of a positive semidefinite quadratic form over the unit cube.

For the co-NP-hardness of containment of an $\mathcal{H}$-polytope in a ball, we provide a reduction from the NP-complete 3-satisfiability problem (3-SAT [5]): Does a given Boolean formula Φ over the variables $z_1, \ldots, z_n$ in conjunctive normal form, where each clause has at most 3 literals, admit an assignment that evaluates TRUE?

The 2^n possible assignments $\{\text{FALSE}, \text{TRUE}\}^n$ for $z_1, \ldots, z_n$ can be identified with the vertices of an n-dimensional cube $[-1, 1]^n$. Let B be a ball (which is a spectrahedron), such that the vertices of $[-1, 1]^n$ just "peak" through its boundary sphere S. Precisely (assuming w.l.o.g. $n \geq 2$), choose the radius r of B such that

$$\left(\frac{1}{6}\right)^2 + \left(\sqrt{n} - \frac{1}{6}\right)^2 \ < \ r^2 \ < \ n\,.$$

Note that such a radius can be determined in polynomial time and size.

For the definition of the $\mathcal{H}$-polytope P, we start from the $\mathcal{H}$-presentation $\{x \in \mathbb{R}^n : -1 \leq x_i \leq 1, 1 \leq i \leq n\}$ of $[-1, 1]^n$ and add one inequality for each clause of Φ. Let $\mathcal{C} = \mathcal{C}_1 \vee \cdots \vee \mathcal{C}_m$ be a 3-SAT formula with clauses $\mathcal{C}_1, \ldots, \mathcal{C}_m$. Denote by $\overline{z_i}$ the complement of a variable z_i, and define the literals $z_i^1 := z_i$, $z_i^0 := \overline{z_i}$. If the clause $\mathcal{C}_i$ is of the form $\mathcal{C}_i = z_{i_1}^{e_{i_1}} \vee z_{i_2}^{e_{i_2}} \vee z_{i_3}^{e_{i_3}}$ with $e_{i_1}, e_{i_2}, e_{i_3} \in \{0, 1\}$ then add the inequality

$$(-1)^{e_{i_1}} x_{i_1} + (-1)^{e_{i_2}} x_{i_2} + (-1)^{e_{i_3}} x_{i_3} \ \leq \ 1\,.$$

If $P \subseteq B$ then, by the choice of r, none of the points in $\{-1, 1\}^n$ can be contained in P and thus there does not exist a valid assignment for Φ. Conversely, assume that P is not contained in B. Let $p \in P \setminus B \subseteq [-1, 1]^n$. We claim that componentwise rounding of p yields an integer point $p' \in \{-1, 1\}^n$ satisfying all defining inequalities of P. To see this, first note that by the choice of the radius of B, the components p_i of p differ at most $\varepsilon < \frac{1}{3\sqrt{2}} < \frac{1}{3}$ from either -1 or 1.

In order to inspect what happens to the inequalities when rounding, assume without loss of generality that the inequality is of the form $x_1 + x_2 + x_3 \geq -1$. We assume a rounded vector p' does not satisfy the inequality, even though p does:

(3.1) $p_1' + p_2' + p_3' \ < \ -1, \quad \text{but } p_1 + p_2 + p_3 \ \geq \ -1\,.$

Since $p' \in \{-1,1\}^n$, (3.1) implies $p'_1 = p'_2 = p'_3 = -1$. Hence, at least one of p_1, p_2 and p_3 differs from either -1 or 1 by more than $1/3$, which is a contradiction. This completes the reduction from 3-SAT.

Finally, deciding whether a spectrahedron S_A is contained in a spectrahedron S_B is co-NP-hard, since already deciding whether an $\mathcal{H}$-polytope is contained in a spectrahedron is co-NP-hard. $\qquad\square$

4. Relaxations and exact cases

In this section, we revisit and extend the relaxation techniques for the containment of spectrahedra from [16]. Our point of departure is the containment problem for pairs of $\mathcal{H}$-polytopes, which by Proposition 3.1 can be decided in polynomial time. Indeed, this can be achieved by solving a linear program, as reviewed by the following necessary and sufficient criterion.

Proposition 4.1. *Let $P_A = \{x \in \mathbb{R}^n : \mathbb{1}_k + Ax \geq 0\}$ and $P_B = \{x \in \mathbb{R}^n : \mathbb{1}_l + Bx \geq 0\}$ be polytopes. There exists a right stochastic matrix C (nonnegative entries, each row summing to one) with $B = CA$ if and only if $P_A \subseteq P_B$.*

For preparing related statements in more general contexts below, we review the proof which uses the following version of Farkas' Lemma:

Proposition 4.2 (Affine form of Farkas' Lemma [28, Corollary 7.1h])**.** *Let the polyhedron $P = \{x \in \mathbb{R}^n : l_i(x) \geq 0, i = 1, \ldots, m\}$ with affine functions $l_i : \mathbb{R}^n \to \mathbb{R}$ be nonempty. Then every affine $l : \mathbb{R}^n \to \mathbb{R}$ that is nonnegative on P can be written as $l(x) = c_0 + \sum_{i=1}^m c_i l_i(x)$ with nonnegative coefficients c_i.*

Proof. (of Proposition 4.1.) If $B = CA$ with a right stochastic matrix C, then for any $x \in P_A$ we have $\mathbb{1}_l + Bx = \mathbb{1}_l + C(Ax) \geq 0$, i.e., $P_A \subseteq P_B$.

Conversely, if $P_A \subseteq P_B$, then for any $i \in \{1, \ldots, l\}$ the i-th row $(\mathbb{1}_l + Bx)_i$ of $\mathbb{1}_l + Bx$ is nonnegative on P_A. Hence, by Proposition 4.2, $(\mathbb{1}_l + Bx)_i$ can be written as a linear combination

$$(\mathbb{1}_l + Bx)_i = 1 + (Bx)_i = c'_{i0} + \sum_{j=1}^k c'_{ij}(\mathbb{1}_k + Ax)_j$$

with nonnegative coefficients c'_{ij}. Comparing coefficients yields $\sum_{j=1}^k c'_{ij} = 1 - c'_{i0}$. Since P_A is a polytope with zero in its interior, the vertices of the polar polytope P_A° are given by the rows $-A_j$ of $-A$. Hence, for every $i \in \{1, \ldots, l\}$ there exists a convex combination $0 = \sum_{j=1}^k \lambda_{ij}(-A_j)$ with nonnegative λ_{ij} and $\sum_{j=1}^k \lambda_{ij} = 1$, which we write as an identity $\sum_{j=1}^k \lambda_{ij}(\mathbb{1}_k + Ax)_j = 1$ of affine functions. By multiplying that equation with c'_{i0}, we obtain nonnegative c''_{ij} with $\sum_{j=1}^k c''_{ij}(\mathbb{1}_k + Ax)_j = c'_{i0}$, which yields

$$1 + (Bx)_i = \sum_{j=1}^k (c'_{ij} + c''_{ij})(\mathbb{1}_k + Ax)_j.$$

Hence, $C = (c_{ij})$ with $c_{ij} := c'_{ij} + c''_{ij}$ is a right stochastic matrix with $B = CA$. $\qquad\square$

The sufficiency part from Proposition 4.1 can be extended to the case of spectrahedra in a natural way. The natural description of a polytope P as a spectrahedron, as introduced in Section 2, is given by

$$P = P_A = \{x \in \mathbb{R}^n \ : \ A(x) = \mathrm{diag}(a_1(x), \ldots, a_k(x)) \succeq 0\},$$

where $a_i(x)$ is the i-th entry of the vector $\mathbb{1}_k + Ax$. Then, as in the definition of a linear pencil (2.2), A_p is the $k \times k$ diagonal matrix $\mathrm{diag}(A_{\cdot,p})$ of the p-th column of A. Proceed in the same way with P_B. Now define a $kl \times kl$ matrix C' by writing the entries of C on the diagonal, i.e. $C' = \mathrm{diag}(c_{11}, \ldots, c_{l1}, c_{12}, \ldots, c_{l2}, \ldots, c_{1k}, \ldots, c_{lk})$. Then the condition from Proposition 4.1 translates to

$$(4.1) \quad C' \text{ diagonal}, \ C' = \left(C'_{ij}\right)_{i,j=1}^{k} \succeq 0, \quad I_l = \sum_{i=1}^{k} C'_{ii}, \quad \forall p = 1, \ldots, n : \ B_p = \sum_{i=1}^{k} a_{ii}^{p} C'_{ii},$$

where a_{ij}^p is the (i,j)-th entry of A_p and $C'_{ij} \in \mathbb{R}^{l \times l}$. Theorem 4.3 below tells us, that C' does not need to be diagonal and yields a sufficient condition for the containment of spectrahedra.

4.1. A sufficient condition for containment of a spectrahedron in a spectrahedron.
Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils.

In the following, the indeterminate matrix $C = (C_{ij})_{i,j=1}^{k}$ ("*Choi matrix*") is a symmetric $kl \times kl$-matrix where the C_{ij} are $l \times l$-blocks. By showing the equivalence of containment of the so-called matricial relaxations of two spectrahedra S_A, S_B given by monic linear pencils and the existence of a completely positive unital linear map $\tau : \mathrm{span}\{A_0, A_1, \ldots, A_n\} \to \mathrm{span}\{B_0, B_1, \ldots, B_n\}$, $A_p \mapsto B_p$, the authors of [15, 16] proved that the system

$$(4.2) \qquad\qquad C = (C_{ij})_{i,j=1}^{k} \succeq 0, \quad \forall p = 0, \ldots, n : \ B_p = \sum_{i,j=1}^{k} a_{ij}^{p} C_{ij}$$

has a solution if and only if the matricial relaxation of S_A is contained in the one of S_B. If so, then $S_A \subseteq S_B$. We show the latter statement in an elementary way, see Theorem 4.3.

Moreover, in our approach it becomes apparent that we can relax the criterion given by Helton, Klep and McCullough by replacing the linear constraint on the constant matrices in (4.2) with semidefinite constraints,

$$(4.3) \quad C = (C_{ij})_{i,j=1}^{k} \succeq 0, \quad B_0 - \sum_{i,j=1}^{k} a_{ij}^{0} C_{ij} \succeq 0, \quad \forall p = 1, \ldots, n : \ B_p = \sum_{i,j=1}^{k} a_{ij}^{p} C_{ij}.$$

This relaxed system is still sufficient for containment of spectrahedra as the following theorem shows.

Theorem 4.3. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils. If one of the systems (4.2) or (4.3) is feasible then $S_A \subseteq S_B$.*

Proof. First we show the statement for (4.3).

For $x \in S_A$, the last two conditions in (4.3) imply

$$(4.4) \quad B(x) = B_0 + \sum_{p=1}^{n} x_p B_p \succeq \sum_{i,j=1}^{k} a_{ij}^0 C_{ij} + \sum_{p=1}^{n} \sum_{i,j=1}^{k} x_p a_{ij}^p C_{ij} = \sum_{i,j=1}^{k} (A(x))_{ij} C_{ij}.$$

Since $A(x)$ and C are positive semidefinite, the Kronecker product $A(x) \otimes C$ is positive semidefinite as well, see (2.1). As a consequence, all principal submatrices of $A(x) \otimes C$ are positive semidefinite. Consider the principal submatrix where we take the (i,j)-th sub-block of every (i,j)-th block,

$$\left((A(x))_{ij} C_{ij} \right)_{i,j=1}^{k} \in \mathcal{S}_{kl}[x].$$

To be more precise, $A(x) \otimes C$ is a $k^2 l \times k^2 l$-matrix with $k \times k$ blocks of the form

$$(A(x))_{ij} C = \begin{bmatrix} (A(x))_{ij} C_{11} & \cdots & (A(x))_{ij} C_{1k} \\ \vdots & (A(x))_{ij} C_{ij} & \vdots \\ (A(x))_{ij} C_{k1} & \cdots & (A(x))_{ij} C_{kk} \end{bmatrix} \in \mathcal{S}_{kl}.$$

(Remember that $(A(x))_{ij}$ is a scalar). Now we take the (i,j)-th block of $(A(x))_{ij} C$, i.e. $(A(x))_{ij} C_{ij}$.

Set $\mathbb{I} = [I_l, \ldots, I_l]^T$. Then the claim for system (4.3) follows from the fact that positive semidefiniteness "$\succeq$" is a transitive relation on the space of symmetric matrices, that is,

$$(4.5) \qquad v^T B(x) v \geq v^T \left(\mathbb{I}^T \left((A(x))_{ij} C_{ij} \right)_{i,j=1}^{k} \mathbb{I} \right) v$$

$$= \left(v^T \ \ldots \ v^T \right) \left((A(x))_{ij} C_{ij} \right)_{i,j=1}^{k} \left(v \ \ldots \ v \right)^T \geq 0$$

for every $v \in \mathbb{R}^l$.

Specializing "$\succeq$" to "$=$" in (4.4) and "$\geq$" to "$=$" in (4.5) provides a streamlined proof for (4.2). $\qquad\square$

For both systems (4.2) and (4.3) the feasibility depends on the linear pencil representation of the sets involved. In Section 6.1 we will take a closer look at this fact.

Remark 4.4. The sub-block argument in the proof of Theorem 4.3 can also be stated in terms of the Khatri-Rao product (see [23]). Let $A = (A_{ij})_{ij}$ and $B = (B_{ij})_{ij}$ be block matrices, consisting of $k \times k$ blocks of size $p \times p$ and $q \times q$, respectively. The *Khatri-Rao product* of A and B is defined as the blockwise Kronecker product of A and B, i.e.,

$$A * B = (A_{ij} \otimes B_{ij})_{ij}.$$

If both A and B are positive semidefinite, then the Khatri-Rao product $A * B$ is positive semidefinite as well, see [23, Theorem 5].

Now consider $A(x)$ and C as in the proof of Theorem 4.3. Then $p = 1$ and $q = l$. Therefore,

$$A(x) * C = ((A(x))_{ij} \otimes C_{ij})_{i,j=1}^{k} = ((A(x))_{ij} C_{ij})_{i,j=1}^{k}$$

is positive semidefinite.

The subsequent statement shows that Theorem 4.3 is invariant under translation. Let S_A be a spectrahedron defined by the linear pencil $A(x) = A_0 + \sum_{p=1}^n x_p A_p$. To move S_A by a vector $v = (v_1, \ldots, v_n)$ we substitute $x - v$ into the pencil and get

$$A(x - v) = A_0 - \sum_{p=1}^n v_p A_p + \sum_{p=1}^n x_p A_p.$$

Lemma 4.5 (Translation symmetry). *The criteria* (4.2) *and* (4.3) *are invariant under translation.*

Proof. Given linear pencils $A(x)$ and $B(x)$, let C be a solution to system (4.3). Then it is also a solution for the translated pencils $A(x - v)$ and $B(x - v)$ for any $v \in \mathbb{R}^n$. The translation only has an impact on the constant matrix, we have to show

$$(4.6) \qquad B_0 - \sum_{p=1}^n v_p B_p - \left(\sum_{i,j=1}^k \left(a_{ij}^0 - \sum_{p=1}^n v_p a_{ij}^p \right) C_{ij} \right) \succeq 0.$$

Since $B_p = \sum_{i,j=1}^k a_{ij}^p C_{ij}$ for all $p = 1, \ldots, n$, (4.6) is equivalent to $B_0 - \sum_{i,j=1}^k a_{ij}^0 C_{ij} \succeq 0$, which is the condition on the constant matrices before translating.

As in the proof of Theorem 4.3, specializing "$\succeq$" to "$=$" yields a proof for (4.2). $\qquad \square$

If S_B is contained in the positive orthant, we can give a stronger version of the criterion introduced in Theorem 4.3.

Corollary 4.6. *Let* $A(x) \in \mathcal{S}_k[x]$ *and* $B(x) \in \mathcal{S}_l[x]$ *be linear pencils and let* S_A *be contained in the positive orthant. If the following system is feasible then* $S_A \subseteq S_B$.

$$(4.7) \quad C = (C_{ij})_{i,j=1}^k \succeq 0, \quad B_0 - \sum_{i,j=1}^k a_{ij}^0 C_{ij} \succeq 0, \quad \forall p = 1, \ldots, n : \ B_p - \sum_{i,j=1}^k a_{ij}^p C_{ij} \succeq 0.$$

Proof. The proof is along the lines of the proof of Theorem 4.3. Indeed, since S_A lies in the positive orthant, we have $x \geq 0$ for all $x \in S_A$ and hence,

$$B(x) = B_0 + \sum_{p=1}^n x_p B_p \ \succeq \ \sum_{i,j=1}^k a_{ij}^0 C_{ij} + \sum_{p=1}^n \sum_{i,j=1}^k x_p \, a_{ij}^p C_{ij} \ = \ \sum_{i,j=1}^k (A(x))_{ij} \, C_{ij}.$$

$$\square$$

By relaxing system (4.2) to (4.7) the number of scalar variables remains $\frac{1}{2}kl(kl + 1)$, whereas the $\frac{1}{2}(n+1)l(l+1)$ linear constraints are replaced by $n+1$ semidefinite constraints of size $l \times l$.

If containment restricted to the positive orthant implies containment everywhere else, criterion (4.7) can be applied, even if the spectrahedron is not completely contained in the positive orthant. To make use of this fact, we have to premise a certain structure of the spectrahedra. We give an example in the following corollary.

Corollary 4.7. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be linear pencils defining spectrahedra with a reflection symmetry with respect to all coordinate hyperplanes. If system (4.7) is feasible then $S_A \subseteq S_B$.*

In Section 6.1 we will see that the relaxed version (4.7) is strictly stronger than system (4.2). There are cases, where a solution to the relaxed problem (4.7) exists, even though the original problem (4.2) is infeasible.

4.2. **Exact cases.** It turns out that the sufficient semidefinite criteria (4.2) and (4.3) even provide exact containment characterizations in several important cases. Detailed statements of these results and their proofs will be given in Statements 4.9, 4.11, 4.13, 5.1.

For ease of notation, most statements in this section as well as in section 5 are given for monic pencils and proved only for criterion (4.2). Note however, that feasibility of (4.2) implies feasibility of (4.3). Furthermore, after translating the (in this section mostly bounded) spectrahedra to the positive orthant, Corollary 4.6 can be applied. Since criterion (4.2) is invariant under translation, its feasibility again implies that system (4.7) has a solution for the translated spectrahedra.

Besides the normal forms of polyhedra, ellipsoids, and balls introduced in Section 2, the exact characterizations will also use the following *extended form* $S_{\widehat{A}}$ of a spectrahedron S_A. Given a linear pencil $A(x) \in \mathcal{S}_k[x]$, we call the linear pencil with an additional 1 on the diagonal

$$(4.8) \qquad \widehat{A}(x) := \begin{bmatrix} 1 & 0 \\ 0 & A(x) \end{bmatrix} \in \mathcal{S}_{k+1}[x]$$

the *extended linear pencil* of $S_A = S_{\widehat{A}}$ (the spectrahedra coincide, only the representations of S_A and $S_{\widehat{A}}$ differ, since the 1 we add for technical reasons is redundant). The entries of $\widehat{A}_p$ in the pencil $\widehat{A}(x) = \widehat{A}_0 + \sum_{p=1}^n x_p \widehat{A}_p$ are denoted by $\widehat{a}_{ij}^p$ for $i, j = 0, \ldots, k$, as usual.

Theorem 4.8. *Let $A(x) \in \mathcal{S}_k[x]$ and $B(x) \in \mathcal{S}_l[x]$ be monic linear pencils. In the following cases the criteria (4.2) as well as (4.3) are necessary and sufficient for the inclusion $S_A \subseteq S_B$:*
   (1) *if $A(x)$ and $B(x)$ are normal forms of ellipsoids (both centrally symmetric, axis-aligned semi-axes),*
   (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 $\widehat{A}(x)$ is the extended form of a spectrahedron and $B(x)$ is the normal form of a polyhedron.*

In this section, we provide the proofs of (1), (2), where the sufficiency parts follow by Theorem 4.3. The cases (3) and (4) will be treated in Section 5. We start with the containment of $\mathcal{H}$-polyhedra in $\mathcal{H}$-polyhedra which slightly generalizes Proposition 4.1 and will be used in the proofs of later statements.

Lemma 4.9. *Let $A(x) \in \mathcal{S}_k[x]$ be the normal form of a polyhedron as defined in (2.3) and let $\widehat{A}(x) = \mathrm{diag}(1, a_1(x), \ldots, a_k(x)) \in \mathcal{S}_{k+1}[x]$ be the extended linear pencil of $A(x)$.*

Let $B(x) \in \mathcal{S}_l[x]$ be the normal form of a polyhedron. When applied to the pencils $\widehat{A}(x)$ and $B(x)$ criterion (4.2) is necessary and sufficient for the inclusion $S_{\widehat{A}} = S_A \subseteq S_B$. If S_A is a polytope, i.e. a bounded polyhedron, the pencil $A(x)$ can be used instead of $\widehat{A}(x)$.

Proof. With regard to (2.3), the polyhedra S_A and S_B are of the form $S_A = \{x \in \mathbb{R}^n : \mathbb{1}_k + Ax \geq 0\}$ and $S_B = \{x \in \mathbb{R}^n : \mathbb{1}_l + Bx \geq 0\}$, respectively, and let $\widehat{A}$ be the $(k+1) \times n$ matrix defined by $\widehat{A} := \begin{bmatrix} 0 \\ A \end{bmatrix}$.

If $S_{\widehat{A}} \subseteq S_B$, then there exist convex combinations $(\mathbb{1}_l + Bx)_i = c_{i0} + \sum_{j=1}^{k} c_{ij}(\mathbb{1}_k + Ax)_j = \sum_{j=0}^{k} c_{ij}(\mathbb{1}_{k+1} + \widehat{A}x)_j$, where $(\mathbb{1}_{k+1} + \widehat{A}x)_0 = 1$ and the coefficients c_{ij} are nonnegative, just as in the proof of Proposition 4.1.

Now we construct a matrix C that is a solution to system (4.2). Recall that C consists of matrices of size $l \times l : C = (C_{st})_{s,t=0}^{k}$. Set the i-th diagonal entry of C_{jj} to be c_{ij}, and choose all other entries to be zero. The resulting matrix is a diagonal matrix with non-negative entries, which makes it positive semidefinite.

Clearly, $B(x) = \sum_{j=0}^{k}(\mathbb{1}_{k+1} + \widehat{A}x)_j C_{jj} = \sum_{i,j=0}^{k}(\mathbb{1}_{k+1} + \widehat{A}x)_j C_{ij}$. Comparing coefficients, we see that $I_l = \sum_{j=0}^{k} C_{jj}$ and $B_p = \sum_{i,j=0}^{k} \widehat{a}_{ij}^p C_{ij}$ for all $p \in \{1, \ldots, n\}$.

If the inner polyhedron S_A is a polytope, the constant 1 is a convex combination of the remaining polynomials $a_1(x), \ldots, a_k(x)$. Thus the additional 1 in the upper left entry of pencil $\widehat{A}(x)$ is not needed. □

As we have seen in the proof of Lemma 4.9, for polyhedra there is a diagonal solution to (4.2). Thus it is sufficient to check the feasibility of the restriction of (4.2) to the diagonal and checking inclusion of polyhedra reduces to a linear program.

Remark 4.10. For unbounded polyhedra, the extended normal form is required in order for the criterion to be exact. Without it, already in the simple case of two half spaces defined by two parallel hyperplanes, system (4.2) is not feasible.

The following statement on ellipsoids uses the normal form (2.4).

Lemma 4.11. *Let two ellipsoids S_A and S_B be centered at the origin with semi-axes parallel to the coordinate axes, given by the normal forms*

$$A(x) = I_{n+1} + \sum_{p=1}^{n} \frac{x_p}{a_p}(E_{p,n+1} + E_{n+1,p}) \text{ and } B(x) = I_{n+1} + \sum_{p=1}^{n} \frac{x_p}{b_p}(E_{p,n+1} + E_{n+1,p}),$$

respectively. Here $(a_1, \ldots, a_n) > 0$ and $(b_1, \ldots, b_n) > 0$ are the vectors of the lengths of the semi-axes. Then system (4.2) is necessary and sufficient for the inclusion $S_A \subseteq S_B$.

Proof. Note first that $k = l = n + 1$. It is obvious that $S_A \subseteq S_B$ if and only if $b_p - a_p \geq 0$ for every $p = 1, \ldots, n$. The matrices underlying the matrix pencils $A(x)$ and $B(x)$ are

$$A_p = \frac{1}{a_p}(E_{p,n+1} + E_{n+1,p}) \text{ and } B_p = \frac{1}{b_p}(E_{p,n+1} + E_{n+1,p})$$

for all $p = 1, \ldots, n$. Now define an $(n+1)^2 \times (n+1)^2$-block matrix C by

$$
(C_{i,j})_{s,t} = \begin{cases} 1 & i = j = s = t, \\ \frac{a_j}{b_j} & i = s = n+1, \ j = t \le n, \\ \frac{a_i}{b_i} & i = s \le n, \ j = t = n+1, \\ \frac{a_i \, a_j}{b_i \, b_j} & i = s \le n, \ j = t \le n, \ i \ne j, \\ 0 & \text{otherwise.} \end{cases}
$$

We show that C is a solution to (4.2). Decompose $x \in \mathbb{R}^{(n+1)^2}$ in blocks of length $n+1$ and write $x_{i,j}$ for the j-th entry in the i-th block. The matrix C is positive semidefinite since

$$
x^T C x = \sum_{i=1}^{n+1} x_{i,i}^2 + 2 \sum_{i<j\le n} \frac{a_i \, a_j}{b_i \, b_j} x_{i,i} x_{j,j} + 2 \sum_{i=1}^{n} \frac{a_i}{b_i} x_{i,i} \, x_{n+1,n+1}
$$

$$
= \left(\sum_{i=1}^{n} \frac{a_i}{b_i} \, x_{i,i} + x_{n+1,n+1} \right)^2 + \sum_{i=1}^{n} \left(1 - \frac{a_i^2}{b_i^2} \right) x_{i,i}^2 \ge 0
$$

for all $x \in \mathbb{R}^{(n+1)^2}$. Clearly, the sum of the diagonal blocks is the identity matrix I_{n+1}. Since every A_p has only two non-zero entries, every B_p is a linear combination of only two blocks of C,

$$
B_p = \frac{1}{a_p} C_{n+1,p} + \frac{1}{a_p} C_{p,n+1}.
$$

This equality is true by the definition of C. $\qquad \square$

Remark 4.12. Using the square matrices E_{ij} of size $(n+1) \times (n+1)$ introduced in Section 2, the matrix C in the proof of Lemma 4.11 has the form

$$
\begin{bmatrix}
E_{1,1} & d_{1,2}E_{1,2} & \cdots & d_{1,n}E_{1,n} & \frac{a_1}{b_1}E_{1,n+1} \\
d_{2,1}E_{2,1} & E_{2,2} & \ddots & \vdots & \vdots \\
\vdots & \ddots & \ddots & d_{n-1,n}E_{n-1,n} & \vdots \\
d_{n,1}E_{n,1} & \cdots & d_{n,n-1}E_{n,n-1} & E_{n,n} & \frac{a_n}{b_n}E_{n,n+1} \\
\frac{a_1}{b_1}E_{n+1,1} & \frac{a_2}{b_2}E_{n+1,2} & \cdots & \frac{a_n}{b_n}E_{n+1,n} & E_{n+1,n+1}
\end{bmatrix},
$$

where $d_{ij} := \frac{a_i \, a_j}{b_i \, b_j}$.

Now we prove exactness of the criterion for the containment of a ball in a polyhedron.

Lemma 4.13. *Let S_A be a ball of radius $r > 0$ in normal form (2.4), and let S_B be a polyhedron in normal form (2.3). For the containment of S_A in S_B, system (4.2) is necessary and sufficient.*

Proof. Note first that $k = n + 1$. Since the normal form $B(x)$ is monic, the linear polynomials describing S_B are of the form $b_i(x) = 1 + \sum_{p=1}^{n} b_{i,p} x_p$ for $i = 1, \ldots, l$. If S_A is contained in the halfspace $b_i(x) \ge 0$, we have $\frac{1}{r^2} \ge \sum_{p=1}^{n} b_{i,p}^2$.

We give a feasible matrix C to system (4.2) to show exactness of the criterion. In this case, C is an $(n+1)l \times (n+1)l$-block matrix defined as follows:

$$(C_{i,j})_{s,t} = \begin{cases} \frac{r^2 b_{s,i}^2}{2} & i = j < k, \ s = t, \\ 1 - \frac{r^2}{2} \sum_{p=1}^n b_{s,i}^2 & i = j = k, \ s = t, \\ \frac{r^2 b_{s,i} b_{s,j}}{2} & i < k, \ j < k, \ i \neq j, \ s = t, \\ \frac{r \, b_{s,j}}{2} & i = k, \ j < k, \ s = t, \\ \frac{r \, b_{s,i}}{2} & j = k, \ i < k, \ s = t, \\ 0 & \text{otherwise.} \end{cases}$$

To show positive semidefiniteness of C, consider a vector $x \in \mathbb{R}^{(n+1)l}$. Decompose x into blocks of length l, and we write $x_{i,j}$ for the j-th entry in the i-th block. Now C is positive semidefinite since

$$x^T C x = \sum_{s=1}^l \left[\sum_{i=j<k} x_{i,s}^2 \frac{r^2 b_{s,i}^2}{2} + x_{k,s}^2 \left(1 - \frac{r^2}{2} \sum_{p=1}^n b_{s,p}^2 \right) \right.$$

$$\left. + 2 \sum_{i<j<k} x_{i,s} x_{j,s} \frac{r^2 b_{s,i} b_{s,j}}{2} + 2 \sum_{i<k} x_{i,s} x_{k,s} \frac{r \, b_{s,i}}{2} \right]$$

$$= \sum_{s=1}^l \left[\left(\sum_{i=j<k} x_{i,s} \frac{r \, b_{s,i}}{\sqrt{2}} + \frac{x_{k,s}}{\sqrt{2}} \right)^2 + \frac{1}{2} x_{k,s}^2 \left(1 - r^2 \sum_{p=1}^n b_{s,p}^2 \right) \right] \geq 0$$

for all $x \in \mathbb{R}^{(n+1)l}$. The term $1 - r^2 \sum_{p=1}^n b_{s,p}^2$ is non-negative since the ball of radius r is contained in S_B and therefore $\frac{1}{r^2} \geq \sum_{p=1}^n b_{s,p}^2$. By construction, the sum of the diagonal blocks is the identity matrix I_l. Every B_p is a linear combination of only two blocks of C,

$$B_p = \frac{1}{r} C_{n+1,p} + \frac{1}{r} C_{p,n+1}.$$

$\square$

Observe that in Lemma 4.9, 4.11 and 4.13 for rational input, C is rational as well.

5. Block diagonalization, transitivity and containment of spectrahedra in polytopes

In [16, Prop. 5.3] Helton, Klep and McCullough showed that the containment criterion (4.2) is exact in an important case, namely if S_B is the cube, given by the monic linear pencil

$$(5.1) \qquad B(x) = I_{2n} + \frac{1}{r} \sum_{p=1}^n x_p \left(E_{pp} - E_{n+p,n+p} \right).$$

The goal in this section is to generalize this to all polyhedra S_B given in normal form (2.3), not only for the original criterion, but also for the variations discussed in Corollaries 4.6

and 4.7. As in Lemma 4.9, in case that S_B is unbounded we have to use the extended normal form $\widehat{A}(x)$ instead of $A(x)$.

Theorem 5.1. *Let $A(x) \in \mathcal{S}_k[x]$ be a monic linear pencil with extended linear pencil $\widehat{A}(x) \in \mathcal{S}_{k+1}[x]$ as defined in equation (4.8) and let $B(x) \in \mathcal{S}_l[x]$ be the normal form of a polyhedron. When applied to the pencils $\widehat{A}(x)$ and $B(x)$ criterion (4.2) is necessary and sufficient for the inclusion $S_{\widehat{A}} = S_A \subseteq S_B$. If S_B is a polytope then the pencil $A(x)$ can be used instead of $\widehat{A}(x)$.*

In order to prove this statement (where the sufficiency-parts are clear from Theorem 4.3) we have to develop some auxiliary results on the behavior of the criterion with regard to block diagonalization and transitivity, which are also of independent interest.

As pointed out by an anonymous referee, this theorem can also be deduced from results of Klep and Schweighofer in [22]. A linear scalar-valued polynomial is positive on a spectrahedron if and only if it is positive on the matricial version of the spectrahedron.

We use the following statement from [16] on the block diagonalization. As usual, for given matrices $M^1, \ldots, M^l$, we denote by the direct sum $\bigoplus_{i=1}^{l} M^i$ the block matrix with diagonal blocks $M^1, \ldots, M^l$ and zero otherwise.

Proposition 5.2. [16, Proposition 4.2] *Let $A(x) \in \mathcal{S}_k[x]$, $B(x) \in \mathcal{S}_l[x]$ and $D^q(x) \in \mathcal{S}_{d_q}[x]$ be linear pencils with $D^q(x) = D_0^q + \sum_{p=1}^{n} x_p D_p^q$, $q = 1, \ldots, m$.*

If $B(x) = \bigoplus_{q=1}^{m} D^q(x)$ is the direct sum with $l = \sum_{q=1}^{m} d_q$, then system (4.2) is feasible if and only if for all $q = 1, \ldots, m$ there exists a $kd_q \times kd_q$-matrix C^q, consisting of $k \times k$ blocks of size $d_q \times d_q$, such that

$$(5.2) \qquad C^q = (C_{ij}^q)_{i,j=1}^{k} \succeq 0, \quad \forall p = 0, \ldots, n: \; D_p^q = \sum_{i,j=1}^{k} a_{ij}^p C_{ij}^q$$

is feasible.
An analogous statement holds for criterion (4.3) and the criteria discussed in Corollaries 4.6 and 4.7.

Since [16] does not contain a proof of this statement, we provide a short one.

Proof. Let $C^1, \ldots, C^m$ be solutions to (5.2), and set $C = \bigoplus_{q=1}^{m} C^q$. Define C' as the direct sum of blocks of C, $C'_{ij} = \bigoplus_{q=1}^{m} C_{ij}^q$. Then C' is a solution to (4.2): C' results by simultaneously permuting rows and columns of C and is thus positive semidefinite. We have $B_p = \bigoplus_{q=1}^{m} D_p^q = \bigoplus_{q=1}^{m} \sum_{i,j=1}^{k} a_{ij} C_{ij}^q = \sum_{i,j=1}^{k} a_{ij} C'_{ij}$.

Conversely, let C' be a solution to (4.2). We are interested in the m diagonal submatrices of each block C'_{ij}, defined as follows: For $q \in \{1, \ldots, m\}$, let $C_{ij}^{\prime q}$ be the $d_q \times d_q$ submatrix of C'_{ij} with row and column indices $\{\sum_{r=1}^{q-1} d_r + 1, \ldots, \sum_{r=1}^{q} d_r\}$. Now the submatrix $C^q = (C_{ij}^{\prime q})_{i,j=1}^{k}$ consisting of the q-th diagonal blocks of each matrix C'_{ij} is a solution to (5.2). C^q is a principal submatrix of C' and thus positive semidefinite. The equations in (5.2) are a subset of the equations in (4.2) and remain valid. $\square$

We now prove transitivity of the containment criterion. We begin with a simple auxiliary lemma on the Kronecker products of corresponding blocks of block matrices.

Lemma 5.3. *Let $A \succeq 0$ consist of $m \times m$ blocks of size $n_a \times n_a$ and $B \succeq 0$ consist of $m \times m$ blocks of size $n_b \times n_b$. Then $\sum_{s,t=1}^{m}(A_{st} \otimes B_{st}) \succeq 0$.*

Proof. First note that we have $v^T \left(\sum_{s,t=1}^{m} A_{st} \right) v = (v^T \ldots v^T)A(v^T \ldots v^T)^T \geq 0$ for all $v \in \mathbb{R}^n$, as in the proof of Theorem 4.3, and hence $\sum_{s,t=1}^{m} A_{st} \succeq 0$.

Since $A, B \succeq 0$, we have $A \otimes B \succeq 0$ as well. $(A_{st} \otimes B_{st})_{s,t=1}^{m}$ is a principal submatrix of this matrix and therefore also positive semidefinite. Summing up the blocks of this matrix and applying our initial considerations, we see that $\sum_{s,t=1}^{m} A_{st} \otimes B_{st} \succeq 0$. ☐

The criteria from Theorem 4.3 are transitive in the following sense.

Theorem 5.4 (Transitivity)**.** *Let $D(x) \in \mathcal{S}_d[x]$, $E(x) \in \mathcal{S}_e[x]$ and $F(x) \in \mathcal{S}_f[x]$ be linear pencils in n variables. If criterion (4.2), criterion (4.3) or criterion (4.7) certifies the inclusion $S_D \subseteq S_E$ and the inclusion $S_E \subseteq S_F$, it also certifies $S_D \subseteq S_F$.*

The transitivity statement concerning (4.2) can be interpreted from an operator theoretic point of view. It states the well-known fact that the composition of two completely positive maps is again completely positive. Our approach enables us to extend the statement to the relaxed criteria (4.3) and (4.7).

Proof. We first consider the relaxed version (4.7). Let C^{DE} be the $de \times de$-matrix certifying the inclusion $S_D \subseteq S_E$ and C^{EF} the $ef \times ef$-matrix certifying the inclusion $S_E \subseteq S_F$. C^{DE} consists of $d \times d$ block matrices of size $e \times e$, C^{EF} consists of $e \times e$ block matrices of size $f \times f$.

We prove that the matrix C^{DF} consisting of $d \times d$ blocks of size $f \times f$ and defined by

$$C_{ij}^{DF} := \sum_{s,t=1}^{e}(C_{ij}^{DE})_{st}C_{st}^{EF}$$

is a solution to system (4.3) for the inclusion $S_D \subseteq S_F$.

To show $C^{DF} \succeq 0$, we start from $C^{DE} \succeq 0$ and $C^{EF} \succeq 0$. Define a new matrix $\tilde{C}^{DE}$ by $(\tilde{C}_{st}^{DE})_{ij} := (C_{ij}^{DE})_{st}$, permuting the rows and columns of C^{DE}. Since rows and columns are permuted simultaneously, positive semidefiniteness is preserved. We think of $\tilde{C}^{DE}$ as having $e \times e$ blocks of size $d \times d$. C^{DF} now simplifies to $C^{DF} = \sum_{s,t=1}^{e} \tilde{C}_{st}^{DE} \otimes C_{st}^{EF}$. Using Lemma 5.3, $C^{DF} \succeq 0$ follows.

Next we show $F_p - \sum_{i,j=1}^{d} d_{ij}^p C_{ij}^{DF} \succeq 0$ for $p = 0, \ldots, n$. By assumption,

$$(5.3) \qquad F_p - \sum_{i,j=1}^{e} e_{ij}^p C_{ij}^{EF} = G^{EF} \succeq 0 \text{ and } E_p - \sum_{i,j=1}^{d} d_{ij}^p C_{ij}^{DE} = G^{DE} \succeq 0.$$

By definition of C^{DF} and the right equation of (5.3), we have

$$\sum_{i,j=1}^{d} d_{ij}^p C_{ij}^{DF} = \sum_{i,j=1}^{d} d_{ij}^p \sum_{s,t=1}^{e} \left(C_{ij}^{DE} \right)_{st} C_{st}^{EF} = \sum_{s,t=1}^{e} \left(E_p - G^{DE} \right)_{st} C_{st}^{EF},$$

and then positive semidefiniteness of G^{EF} and G^{DE} yield

$$F_p - \sum_{i,j=1}^{d} d_{ij}^p C_{ij}^{DF} = G^{EF} + \sum_{s,t=1}^{e} G_{st}^{DE} C_{st}^{EF} \succeq 0\,.$$

The non-relaxed version (4.2) as well as the relaxed version (4.3) follow by choosing G^{EF} and G^{DE} in (5.3) to be zero matrices. □

We can now establish the proof of Theorem 5.1, which also completes the proof of Theorem 4.8.

Proof. (of Theorem 5.1.) Every (monic) linear pencil $B(x)$ in normal form (2.3) can be stated as a direct sum

$$B(x) = \bigoplus_{q=1}^{l} b^q(x) = \bigoplus_{q=1}^{l} (\mathbb{1}_l + Bx)_q.$$

Therefore, Proposition 5.2 implies that system (4.2) is feasible if and only if the system

$$C^q = (C_{ij})_{i,j=1}^{k} \succeq 0, \quad 1 = \sum_{i=1}^{k} C_{ii}^q, \quad \forall p = 1, \dots, n: \ b_p^q = \sum_{i,j=1}^{k} a_{ij}^p C_{ij}^q$$

is feasible for all $q = 1, \dots, l$. Note that C^q is in $\mathcal{S}_k$. Hence, the system has the form

(5.4) $\quad C^q = (C_{ij})_{i,j=1}^{k} \succeq 0, \quad 1 = \langle I_k, C^q \rangle, \quad \forall p = 1, \dots, n: \ b_p^q = \langle A_p, C^q \rangle\,.$

In the following, we show the existence of a solution by duality theory of semidefinite programming and transitivity of (4.2), see Theorem 5.4.

Let $b_1^q, \dots, b_n^q$ be the coefficients of the linear form $b^q(x) = (\mathbb{1}_l + Bx)_q$. Since $B(x)$ is in normal form (2.3), the vector $b^q := (b_1^q, \dots, b_n^q)$ is an inner normal vector to the hyperplane $b^q(x) = 0$. Consider the semidefinite program

(P_q)
$$r_q := \max \ \langle -b^q, x \rangle$$
$$\text{s.t. } A(x) \succeq 0$$

for all $q = 1, \dots, l$. By assumption, (P_q) is strictly feasible and the optimal value is finite. Hence (see, e.g., [6, Thm. 2.2]), the dual problem

(D_q)
$$\min \ \langle I_k, Y^q \rangle$$
$$\text{s.t. } \langle A_p, Y^q \rangle = b_p^q \quad \forall p = 1, \dots, n,$$
$$Y^q \succeq 0$$

has the same optimal value and attains it. (Note that by duality $\langle -A_p, Y^q \rangle = -b_p^q$.) We can scale the primal and dual problems simultaneously by dividing by r_q and get

$(\tilde{D}_q)$
$$1 = \min \ \langle I_k, \tilde{Y}^q \rangle$$
$$\text{s.t. } \langle A_p, \tilde{Y}^q \rangle = \frac{b_p^q}{r_q} \quad \forall p = 1, \dots, n,$$
$$\tilde{Y}^q \succeq 0,$$

in which $\tilde{Y}^q := \frac{Y_q}{r_q}$.

Since in the dual (D_q) the optimal value is attained, in $(\tilde{D}_q)$ it is as well, i.e., for all $q = 1, \ldots, l$ there exists a $k \times k$-matrix C^q such that

$$C^q \succeq 0, \quad 1 = \langle I_k, C^q \rangle, \quad \frac{b_p^q}{r_q} = \langle A_p, C^q \rangle.$$

As mentioned before (5.4), the matrices C^q certify the inclusion $S_A \subseteq S_{B'}$, where $B'(x)$ is defined as the scaled monic linear pencil

$$B'(x) = \bigoplus_{q=1}^{l} \left(1 + \sum \frac{b_p^q}{r_q} x_p \right).$$

Now we have to distinguish between the two cases in the statement of the theorem.

First consider the case where S_B is a polytope. Since $B(x)$ is in normal form, we have $\max_{x \in S_B} \langle -b^q, x \rangle = 1$. Further, since $S_A \subseteq S_B$, the definition of r_q implies $r_q \le 1$ and hence, $S_{B'} \subseteq S_B$. By transitivity and by exactness of the criterion for polytopes, see Theorem 5.4 and Lemma 4.9, respectively, there is a solution of system (4.2) that certifies $S_A \subseteq S_B$.

To prove the unbounded case in the theorem, we construct a solution to (4.2) for the inclusion $S_{\widehat{A}} \subseteq S_{\widehat{B'}}$, where $\widehat{B'}(x) = 1 \oplus B'(x)$ denotes the extended normal form (4.8) of the polyhedron $S_{B'}$. Then the claim follows by Lemma 4.9 and Theorem 5.4, as above, since $S_{\widehat{B'}} \subseteq S_{B'}$ is certified by (4.2).

First note that $S_{\widehat{A}} \subseteq S_B$ is equivalent to $S_A \subseteq S_B$. Denote by C' the matrix that certifies the inclusion $S_A \subseteq S_{B'}$. Then the symmetric $(k+1)(l+1) \times (k+1)(l+1)$-matrix

$$\widehat{C} := E_{11} \oplus \left[\begin{array}{cc} 0 & 0 \\ 0 & C'_{ij} \end{array} \right]_{i,j=1}^{k},$$

where E_{11} and the blocks $\left[\begin{array}{cc} 0 & 0 \\ 0 & C'_{ij} \end{array} \right]_{i,j=1}^{k}$ are of size $(l+1) \times (l+1)$, certifies the inclusion $S_{\widehat{A}} \subseteq S_{\widehat{B'}}$. Indeed, adding zero-columns and zero-rows simultaneously preserves positive semidefiniteness and, clearly, the sum of the diagonal blocks of $\widehat{C}$ is the identity matrix I_{l+1}. Since in every $\widehat{A}_p$ the first column and the first row are the zero vector, we get

$$\sum_{i,j=0}^{k} \widehat{a}_{ij}^p \widehat{C}_{ij} = 0 \cdot E_{11} + \left[\begin{array}{cc} 0 & 0 \\ 0 & \sum_{i,j=1}^{k} a_{ij}^p C'_{ij} \end{array} \right] = \widehat{B'}_p,$$

where $\widehat{a}_{ij}^p$ is the (i, j)-th entry of $\widehat{A}_p$.

Feasibility of the relaxed criteria is again implied by the feasibility of (4.2). $\qquad \square$

6. Containment of scaled spectrahedra and inexact cases

Contrasting the results of Sections 4 and 5, we first consider a situation where the containment criterion fails and the relaxed version (4.7) is strictly stronger. In particular, this raises the question whether (for a spectrahedron S_A contained in a spectrahedron S_B)

the criterion becomes satisfied when scaling S_A by a suitable factor. In Proposition 6.2, we answer this question in the affirmative. We then close the paper by applying this result on optimization versions of the containment problem.

6.1. **Cases where the criterion fails.** We review an example from [16, Example 3.1, 3.4] which shows that the containment criterion is not exact in general. We then contrast this phenomenon by showing that for this example there exists a scaling factor r for one of the spectrahedra so that the containment criterion is satisfied after this scaling.

Consider the monic linear pencils $A(x) = I_3 + x_1(E_{1,3} + E_{3,1}) + x_2(E_{2,3} + E_{3,2}) \in \mathcal{S}_3[x]$ and

$$B(x) = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} + x_1 \begin{bmatrix} 1 & \\ & -1 \end{bmatrix} + x_2 \begin{bmatrix} & 1 \\ 1 & \end{bmatrix}.$$

Clearly, both define the unit disc, that is $S_A = S_B$.

Claim. The containment question $S_B \subseteq S_A$ is certified by criterion (4.2), while the reverse containment question $S_A \subseteq S_B$ is not certified by the criterion.

First, we look into the inclusion $S_B \subseteq S_A$ (where the roles of A and B in (4.2) have to be interchanged). Criterion (4.2) is satisfied if and only if there exist $c_1, c_2, c_3 \in \mathbb{R}$ such that

$$C = \left[\begin{array}{ccc|ccc} \frac{1}{2} & 0 & \frac{1}{2} & 0 & c_1 & c_2 \\ 0 & \frac{1}{2} & 0 & -c_1 & 0 & c_3 \\ \frac{1}{2} & 0 & \frac{1}{2} & -c_2 & 1-c_3 & 0 \\ \hline 0 & -c_1 & -c_2 & \frac{1}{2} & 0 & -\frac{1}{2} \\ c_1 & 0 & 1-c_3 & 0 & \frac{1}{2} & 0 \\ c_2 & c_3 & 0 & -\frac{1}{2} & 0 & \frac{1}{2} \end{array} \right] \in \mathbb{R}^{6\times 6}$$

is positive semidefinite. Since the 2×2-block in the top left corner is positive definite, the matrix C is positive semidefinite if and only if the Schur complement with respect to this block is positive semidefinite. One can easily check that this is the case if and only if $c_1 = c_3 = \frac{1}{2}$ and $c_2 = 0$.

Conversely, $S_A \subseteq S_B$ is certified by (4.2) if and only if there exist $c_1, \ldots, c_{12} \in \mathbb{R}$ such that

$$C = \left[\begin{array}{cc|cc|cc} c_1 & c_2 & c_9 & c_{10} & \frac{1}{2} & c_7 \\ c_2 & c_3 & c_{11} & c_{12} & -c_7 & -\frac{1}{2} \\ \hline c_9 & c_{11} & c_4 & c_5 & 0 & c_8 \\ c_{10} & c_{12} & c_5 & c_6 & 1-c_8 & 0 \\ \hline \frac{1}{2} & -c_7 & 0 & 1-c_8 & 1-c_1-c_4 & -c_2-c_5 \\ c_7 & -\frac{1}{2} & c_8 & 0 & -c_2-c_5 & 1-c_3-c_6 \end{array} \right] \in \mathbb{R}^{6\times 6}$$

is positive semidefinite. We show the infeasibility of the system (4.2).

Assume that C is positive semidefinite. Then all principal minors are non-negative. Consider the principal minor

$$\begin{vmatrix} c_1 & \frac{1}{2} \\ \frac{1}{2} & 1-c_1-c_4 \end{vmatrix} = c_1(1-c_1-c_4) - \frac{1}{4} = \left[c_1(1-c_1) - \frac{1}{4} \right] - c_1 c_4.$$

Since the expression in the brackets as well as the second term are always less than or equal to zero the minor is non-positive. Therefore, $c_1(1 - c_1) - \frac{1}{4} = 0$ and $c_1 c_4 = 0$, or equivalently, $c_1 = \frac{1}{2}$ and $c_4 = 0$.

Recall that whenever a diagonal element of a positive semidefinite matrix is zero, the corresponding row is the zero vector, that is $c_5 = c_8 = c_9 = c_{11} = 0$. Now, we get a contradiction since the principal minor

$$\begin{vmatrix} c_6 & 1 - c_8 \\ 1 - c_8 & 1 - c_1 - c_4 \end{vmatrix} = \begin{vmatrix} c_6 & 1 \\ 1 & \frac{1}{2} \end{vmatrix} = \frac{1}{2} c_6 - 1$$

implies that $c_6 \geq 2$ and therefore $1 - c_3 - c_6 \leq -1 - c_3 < 0$ or $c_3 < -1$. This proves the claim.

Now, generalizing $A(x)$, let $A^r(x)$ be the linear pencil of the ball with radius $(1 >)r > 0$ in normal form. With regard to the containment question $S_{A^r} = rS_A \subseteq S_B$, we show the feasibility of system (4.2) for r sufficiently small. Consider the matrix

$$C = \left[\begin{array}{cc|cc|cc} c & 0 & 0 & c & \frac{r}{2} & 0 \\ 0 & c & -c & 0 & 0 & -\frac{r}{2} \\ \hline 0 & -c & c & 0 & 0 & \frac{r}{2} \\ c & 0 & 0 & c & \frac{r}{2} & 0 \\ \hline \frac{r}{2} & 0 & 0 & \frac{r}{2} & 1 - 2c & 0 \\ 0 & -\frac{r}{2} & \frac{r}{2} & 0 & 0 & 1 - 2c \end{array} \right] \in \mathbb{R}^{6 \times 6}.$$

Obviously the equality constraints in (4.2) are fulfilled.

As above, if $c = 0$ or $1 - 2c = 0$, then $r = 0$. Therefore, $0 < c < \frac{1}{2}$ and the 2×2-block in the top left corner C_{11} is positive definite. Thus the matrix C is positive semidefinite if and only if the Schur complement with respect to C_{11} is positive semidefinite. This is the case if and only if

$$1 - 2c - \frac{r^2}{4c} \geq 0 \iff f(c) := 8c^2 - 4c + r^2 \leq 0.$$

Assume $r > \frac{1}{2}\sqrt{2}$. Then $f(c) > 0$ for all c since f has no real roots and the constant term $f(0) = r^2$ is positive. Otherwise, $f(\frac{1}{4}) = -\frac{1}{2} + r^2 \leq 0$. Hence, system (4.2) is feasible for $0 < r \leq \frac{1}{2}\sqrt{2}$.

The problem of maximizing r such that the system (4.2) is feasible can be formulated as a semidefinite program. A numerical computation yields an optimal value of $0.707 \approx \frac{1}{2}\sqrt{2}$.

Note that we are in the situation of Corollary 4.7. For the relaxed version (4.7), a numerical computation gives the optimal value of $0.950 \approx \frac{19}{20}$. In particular, this shows that the relaxed criterion (4.7) can be satisfied in cases where the non-relaxed criterion (4.2) does not certify an inclusion.

It is an open research question to establish a quantitative relationship comparing criterion (4.7) to (4.2) in the general case.

6.2. **Containment of scaled spectrahedra.** For a monic linear pencil $A(x) \in \mathcal{S}_k[x]$ and a constant $\nu > 0$ define

$$(6.1) \qquad A^\nu(x) := A\left(\frac{x}{\nu}\right) = I_k + \frac{1}{\nu} \sum_{p=1}^{n} x_p A_p,$$

the ν-scaled (monic linear) pencil. Similarly, we denote by $\nu S_A := \{x \in \mathbb{R}^n : A^\nu(x) \succeq 0\}$ the corresponding ν-scaled spectrahedron.

Generalizing the observation from Section 6.1, we show that for two spectrahedra S_A and S_B, containing the origin in their interior, there always exists some scaling factor ν such that the criteria (4.2) and (4.3) certify the inclusion $\nu S_A \subseteq S_B$. This extends the following result of Ben-Tal and Nemirovski, who treated containment of a cube in a spectrahedron (in which case they can even give a bound on the scaling factor).

Proposition 6.1. [2, Thm. 2.1] *Let S_A be the cube (5.1) with edge length $r > 0$ and consider a monic linear pencil $B(x)$. Let $\mu = \max_{p=1,\dots,n} \operatorname{rank} B_p$. If $S_A \subseteq S_B$, then system (4.2) is feasible for the $\nu(\mu)$-scaled cube $\nu(\mu)S_A$, where $\nu(\mu)$ is given by*

$$\nu(\mu) = \min_{y \in \mathbb{R}^\mu, \|y\|_1 = 1} \left\{ \int_{\mathbb{R}^\mu} \left| \sum_{i=1}^{\mu} y_i u_i^2 \right| \left(\frac{1}{2\mu}\right)^{\frac{\mu}{2}} \exp\left(-\frac{u^T u}{2}\right) du \right\}.$$

For all μ the bound $\nu(\mu) \geq \frac{2}{\pi\sqrt{\mu}}$ holds.

A quantitative result as presented in the last Proposition is not known for the general case. However, combining Proposition 6.1 with our results from Sections 4 and 5 we get that for spectrahedra with non-empty interior, there is always a scaling factor such that system (4.2) and thus also system (4.3) hold.

Proposition 6.2. *Let $A(x)$ and $B(x)$ be monic linear pencils such that S_A is bounded. Then there exists a constant $\nu > 0$ such that for the scaled spectrahedron νS_A the inclusion $\nu S_A \subseteq S_B$ is certified by the systems (4.2) and (4.3).*

We provide a proof based on the framework established in the previous sections. Alternatively it can be deduced from statements about the matricial relaxation of criterion (4.2) given in the work by Helton and McCullough [17], see also [16]. Criterion (4.2) is satisfied for linear pencils $A^\nu(x)$ and $B(x)$ if and only if the matricial version of νS_A is contained in the matricial version of S_B.

Proof. Denote by S_D the cube, defined by the monic linear pencil (5.1), with the minimal edge length such that S_A is contained in it, which can be computed by a semidefinite program, see Theorem 5.1. Since $B(x)$ is monic, there is an open subset around the origin contained in S_B. Thus there is a scaling factor $\nu_1 > 0$ so that $\nu_1 S_A \subseteq \nu_1 S_D \subseteq S_B$.

By Proposition 6.1, there exists a constant $\nu_2 > 0$ such that for the problem $\nu_2\nu_1 S_D \subseteq S_B$ system (4.2) has a solution $C^{D^\nu B}$ with $\nu = \nu_1\nu_2$. By Theorem 5.1, there is a matrix $C^{A^\nu D^\nu}$ which solves (4.2) for the problem νS_A in νS_D.

Finally, Theorem 5.4 implies the feasibility of system (4.2) with respect to νS_A and S_B by the matrix $C^{A^\nu B}$, as defined there. $\square$

In the proof of Proposition 6.2, we scaled the spectrahedron S_A by a certain factor ν. Since $\nu S_A \subseteq S_B$ is equivalent to $S_A \subseteq \frac{1}{\nu} S_B$, the criterion (4.2) remains a positive semidefinite condition even in the presence of the factor ν. Moreover, we can optimize for ν such that the criterion remains satisfied. Proposition 6.2 implies that for bounded spectrahedra represented by monic linear pencils the maximization problem for ν always has a positive optimal value.

This yields a natural framework for the approximation of smallest enclosing spectrahedra and largest enclosed spectrahedra. In [16, Section 4], the example of computing a bound for the norm of the elements of a spectrahedron S_A (represented by a monic linear pencil) is given. This can be achieved by choosing S_B to be the ball centered at the origin, see (2.4).

As we have seen in Section 6.1, applying criterion (4.7) to the problem is stronger than specializing criterion (4.2) to it. However, for the criterion (4.2), we obtain a particularly nice representation, it reduces to the semidefinite system

$$C = (C_{ij})_{i,j=1}^{k} \succeq 0,$$

$$I_{n+1} = \sum_{i=1}^{k} C_{ii},$$

(6.2)

$$\forall p = 1, \ldots, n, \ \forall (s,t) \in \{1, \ldots, n+1\}^2 :$$

$$\left(\sum_{i,j=1}^{k} a_{ij}^p C_{ij} \right)_{st} = \begin{cases} \frac{1}{r} & \text{if } (s,t) \in \{(p, n+1), (n+1, p)\}, \\ 0 & \text{else.} \end{cases}$$

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