NEW APPROXIMATIONS FOR THE CONE OF COPOSITIVE MATRICES AND ITS DUAL

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Abstract. We provide convergent hierarchies for the cone $\mathcal{C}$ of copositive matrices and its dual, the cone of completely positive matrices. In both cases the corresponding hierarchy consists of nested spectrahedra and provide outer (resp. inner) approximations for $\mathcal{C}$ (resp. for its dual $\mathcal{C}^*$), thus complementing previous inner (resp. outer) approximations for $\mathcal{C}$ (for $\mathcal{C}^*$). In particular, both inner and outer approximations have a very simple interpretation. Finally, extension to $\mathcal{K}$-copositivity and $\mathcal{K}$-complete positivity for a closed convex cone $\mathcal{K}$, is straightforward.

1. Introduction

In recent years the cone $\mathcal{C}$ of *copositive* matrices and its dual cone $\mathcal{C}^*$ of *completely positive* matrices have attracted a lot of attention, in part because several interesting NP-hard problems can be modelled as convex conic optimization problems over those cones. For a survey of results and discussion on $\mathcal{C}$ and its dual, the interested reader is referred to e.g. Anstreicher and Burer [1], Burer [3], Dür [6] and Hiriart-Urruty and Seeger [7]..

As optimizing over $\mathcal{C}$ (or its dual) is in general difficult, a typical approach is to optimize over simpler and more tractable cones. In particular, nested hierarchies of tractable convex cones $\mathcal{C}_k$, $k \in \mathbb{N}$, that provide *inner* approximations of $\mathcal{C}$ have been proposed, notably by Parrilo [9], deKlerk and Pasechnik [5], Bomze and deKlerk [2], as well as Peña et al. [10]. For example, denoting by $\mathcal{N}$ (resp. $\mathcal{S}_+$) the convex cone of nonnegative (resp. positive semidefinite) matrices, the first cone in the hierarchy of [5] is $\mathcal{N}$, and $\mathcal{N} + \mathcal{S}_+$ in that of [9], whereas the hierarchy of [10] is in sandwich between that of [5] and [9]. Of course, to each such hierarchy of inner approximations $(\mathcal{C}_k)$, $k \in \mathbb{N}$, of $\mathcal{C}$, one may associate the hierarchy $(\mathcal{C}_k^*)$, $k \in \mathbb{N}$, of dual cones which provides outer approximations of $\mathcal{C}^*$.

However, quoting Dür in [6]: "We are not aware of comparable approximation schemes that approximate the completely positive cone (i.e. $\mathcal{C}^*$) from the interior."

The contribution of this note is precisely to describe an explicit hierarchy of tractable convex cones that provide *outer* approximations of $\mathcal{C}$ and so, by duality, the corresponding hierarchy of dual cones provides *inner* approximations of $\mathcal{C}^*$, answering Dür's question and also showing that $\mathcal{C}$ and $\mathcal{C}^*$ can be sandwiched between two converging hierarchies of tractable convex cones. This result is a consequence of a more general result of [8] about nonnegativity on a closed set $\mathbf{K} \subset \mathbb{R}^n$. However,

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its specialization to the present context of $\mathbf{K} = \mathcal{C}$ (or $\mathcal{C}^*$) yields inner approximations for $\mathcal{C}^*$ with a very simple interpretation directly related to the definition of $\mathcal{C}^*$, which might be of interest for the community interested in $\mathcal{C}$ and $\mathcal{C}^*$ but might be "lost" in the general case treated in [8], whence the present note. Finally, following Burer [3], and $\mathcal{K} \subset \mathbb{R}^n$ being a closed convex cone, one may also consider the convex cone $\mathcal{C}_{\mathcal{K}}$ of $\mathcal{K}$-copositive matrices, i.e., real symmetric matrices $\mathbf{A}$ such that $\mathbf{x}^T\mathbf{A}\mathbf{x} \geq 0$ on $\mathcal{K}$, and its dual cone $\mathcal{C}^*_{\mathcal{K}}$ of $\mathcal{K}$-completely positive matrices. Then the outer approximations previously defined have an immediate and straightforward analogue (as well as the inner approximations of the dual).

2. Main result

2.1. **Notation and definition.** Let $\mathbb{R}[\mathbf{x}]$ be the ring of polynomials in the variables $\mathbf{x} = (x_1, \ldots, x_n)$. Denote by $\mathbb{R}[\mathbf{x}]_d \subset \mathbb{R}[\mathbf{x}]$ the vector space of polynomials of degree at most d, which forms a vector space of dimension $s(d) = \binom{n+d}{d}$, with e.g., the usual canonical basis $(\mathbf{x}^\alpha)$ of monomials. Also, denote by $\Sigma[\mathbf{x}] \subset \mathbb{R}[\mathbf{x}]$ (resp. $\Sigma[\mathbf{x}]_d \subset \mathbb{R}[\mathbf{x}]_{2d}$) the space of sums of squares (s.o.s.) polynomials (resp. s.o.s. polynomials of degree at most $2d$). If $f \in \mathbb{R}[\mathbf{x}]_d$, write $f(\mathbf{x}) = \sum_{\alpha\in\mathbb{N}^n} f_\alpha \mathbf{x}^\alpha$ in the canonical basis and denote by $\mathbf{f} = (f_\alpha) \in \mathbb{R}^{s(d)}$ its vector of coefficients. Finally, let $\mathcal{S}^n$ denote the space of $n \times n$ real symmetric matrices, with inner product $\langle \mathbf{A}, \mathbf{B}\rangle = \mathrm{trace}\,\mathbf{AB}$, and where the notation $\mathbf{A} \succeq 0$ (resp. $\mathbf{A} \succ 0$) stands for $\mathbf{A}$ is positive semidefinite.

Given $\mathbf{K} \subseteq \mathbb{R}^n$, denote by $\mathrm{cl}\,\mathbf{K}$ (resp. $\mathrm{conv}\,\mathbf{K}$) the closure (resp. the convex hull) of $\mathbf{K}$. Recall that given a convex cone $\mathbf{K} \subseteq \mathbb{R}^n$, the convex cone $\mathbf{K}^* = \{\mathbf{y} \in \mathbb{R}^n : \langle \mathbf{y}, \mathbf{x}\rangle \geq 0\; \forall \mathbf{x} \in \mathbf{K}\}$ is called the *dual* cone of $\mathbf{K}$, and satisfies $(\mathbf{K}^*)^* = \mathrm{cl}\,\mathbf{K}$. Moreover, given two convex cones $\mathbf{K}_1, \mathbf{K}_2 \subseteq \mathbb{R}^n$,

$$\begin{array}{rclcl} \mathbf{K}_1^* \cap \mathbf{K}_2^* &=& (\mathbf{K}_1 + \mathbf{K}_2)^* &=& (\mathbf{K}_1 \cup \mathbf{K}_2)^* \\ (\mathbf{K}_1 \cap \mathbf{K}_2)^* &=& \mathrm{cl}\,(\mathbf{K}_1^* + \mathbf{K}_2^*) &=& \mathrm{cl}\,(\mathrm{conv}\,(\mathbf{K}_1^* \cup \mathbf{K}_2^*)\,). \end{array}$$

See for instance Dattorro [4, p. 163–164].

Moment matrix. With a sequence $\mathbf{y} = (y_\alpha)$, $\alpha \in \mathbb{N}^n$, let $L_\mathbf{y} : \mathbb{R}[\mathbf{x}] \to \mathbb{R}$ be the linear functional

$$h \quad (= \sum_\alpha h_\alpha \mathbf{x}^\alpha) \quad \mapsto \quad L_\mathbf{y}(h) = \sum_\alpha h_\alpha\, y_\alpha, \quad h \in \mathbb{R}[\mathbf{x}].$$

With $d \in \mathbb{N}$, let $\mathbb{N}^n_d := \{\alpha \in \mathbb{N}^n : \sum_i \alpha_i \leq d\}$, and let $\mathbf{M}_d(\mathbf{y})$ be the symmetric matrix with rows and columns indexed $\mathbb{N}^n_d$, and defined by:

$$\mathbf{M}_d(\mathbf{y})(\alpha,\beta) := L_\mathbf{y}(\mathbf{x}^{\alpha+\beta}) = y_{\alpha+\beta}, \quad \alpha,\beta \in \mathbb{N}^n_d. \tag{2.1}$$

The matrix $\mathbf{M}_d(\mathbf{y})$ is called the moment matrix associated with $\mathbf{y}$, and it is straightforward to check that

$$\left[\, L_\mathbf{y}(g^2) \geq 0 \quad \forall g \in \mathbb{R}[\mathbf{x}]\,\right] \quad \Leftrightarrow \quad \mathbf{M}_d(\mathbf{y}) \succeq 0, \quad d = 0, 1, \ldots.$$

Localizing matrix. Similarly, with $\mathbf{y} = (y_\alpha)$, $\alpha \in \mathbb{N}^n$, and $f \in \mathbb{R}[\mathbf{x}]$ written

$$\mathbf{x} \mapsto f(\mathbf{x}) = \sum_{\gamma\in\mathbb{N}^n} f_\gamma\, \mathbf{x}^\gamma,$$

let $\mathbf{M}_d(f\,\mathbf{y})$ be the symmetric matrix with rows and columns indexed in $\mathbb{N}^n_d$, and defined by:

$$\mathbf{M}_d(f\,\mathbf{y})(\alpha,\beta) \,:=\, L_{\mathbf{y}}\left(f(\mathbf{x})\,\mathbf{x}^{\alpha+\beta}\right) \,=\, \sum_{\gamma} f_\gamma\, y_{\alpha+\beta+\gamma}, \qquad \forall\,\alpha,\beta\in\mathbb{N}^n_d. \tag{2.2}$$

The matrix $\mathbf{M}_d(f\,\mathbf{y})$ is called the localizing matrix associated with $\mathbf{y}$ and $f\in\mathbb{R}[\mathbf{x}]$. Observe that

$$\langle \mathbf{g}, \mathbf{M}_d(f\,\mathbf{y})\mathbf{g}\rangle \,=\, L_{\mathbf{y}}(g^2\,f), \qquad \forall g\in\mathbb{R}[\mathbf{x}]_d, \tag{2.3}$$

and so if $\mathbf{y}$ has a representing finite Borel measure μ, i.e., if

$$y_\alpha \,=\, \int \mathbf{x}^\alpha\, d\mu, \qquad \forall\,\alpha\in\mathbb{N}^n,$$

then (2.3) reads

$$\langle \mathbf{g}, \mathbf{M}_d(f\,\mathbf{y})\mathbf{g}\rangle \,=\, L_{\mathbf{y}}(g^2\,f) \,=\, \int g(\mathbf{x})^2 f(\mathbf{x})\,d\mu(\mathbf{x}), \qquad \forall g\in\mathbb{R}[\mathbf{x}]_d. \tag{2.4}$$

Actually, the localizing matrix $\mathbf{M}_d(f\,\mathbf{y})$ is nothing less than the moment matrix associated with the sequence $\mathbf{z} = f\,\mathbf{y} = (z_\alpha)$, $\alpha\in\mathbb{N}^n$, with $z_\alpha = \sum_\gamma f_\gamma y_{\alpha+\gamma}$. In particular, if f is nonnegative on the support $\mathrm{supp}\,\mu$ of μ then the localizing matrix $\mathbf{M}_d(f\,\mathbf{y})$ is just the moment matrix associated with the finite Borel measure $d\mu_f = f d\mu$, absolutely continuous with respect to μ (denoted $\mu_f \ll \mu$), and with density f. For instance, with $d=1$ one may write

$$\mathbf{M}_1(f\,\mathbf{y}) \,=\, \int \left[\begin{array}{ccc} 1 & | & \mathbf{x}^T \\ - & & - \\ \mathbf{x} & | & \mathbf{x}\mathbf{x}^T \end{array}\right] f(\mathbf{x})\,d\mu(\mathbf{x}) \,=\, \int \left[\begin{array}{ccc} 1 & | & \mathbf{x}^T \\ - & & - \\ \mathbf{x} & | & \mathbf{x}\mathbf{x}^T \end{array}\right] d\mu_f(\mathbf{x}),$$

or, equivalently,

$$\mathbf{M}_1(f\,\mathbf{y}) \,=\, \mathrm{mass}(\mu)\times \left[\begin{array}{ccc} 1 & | & \mathrm{E}_{\mu_f}(\mathbf{x})^T \\ - & & - \\ \mathrm{E}_{\mu_f}(\mathbf{x}) & | & \mathbf{M}^2_1(f\,\mathbf{y}) \end{array}\right], \tag{2.5}$$

where E_{μ_f} denotes the expectation operator associated with the normalisation $\tilde{\mu}_f$ of μ_f, and $\mathbf{M}^2_1(f\,\mathbf{y})$ denotes the covariance matrix of $\tilde{\mu}_f$.

2.2. **Main result.** With $\mathbf{A} = (a_{ij}) \in \mathcal{S}^n$, let denote by $f_{\mathbf{A}}\in\mathbb{R}[\mathbf{x}]$ the polynomial associated with the quadratic form $\mathbf{x}\mapsto\mathbf{x}^T\mathbf{A}\mathbf{x}$, and let μ be the exponential probability measure supported on $\mathbb{R}^n_+$, and with moments $\mathbf{y}=(y_\alpha)$, $\alpha\in\mathbb{N}^n$ given by:

$$y_\alpha \,=\, \int_{\mathbb{R}^n_+} \exp\left(-\sum_{i=1}^n x_i^{\alpha_i}\right)\,d\mu(\mathbf{x}) \,=\, \prod_{i=1}^n \frac{1}{\alpha_i!}, \qquad \forall\,\alpha\in\mathbb{N}^n. \tag{2.6}$$

Recall that a matrix $\mathbf{A}\in\mathcal{S}^n$ is copositive if $f_{\mathbf{A}}(\mathbf{x})\geq 0$ for all $\mathbf{x}\in\mathbb{R}^n_+$, and denote by $\mathcal{C}\subset\mathcal{S}^n$ the cone of copositive matrices, i.e.,

$$\mathcal{C} \,:=\, \{\,\mathbf{A}\in\mathcal{S}^n \,:\, f_{\mathbf{A}}(\mathbf{x}) \,\geq\, 0 \quad \forall\,\mathbf{x}\geq 0\,\}. \tag{2.7}$$

Its dual cone is the closed convex cone of *completely positive*, i.e., matrices of $\mathcal{S}^n$ that can be written as the sum of finitely many rank-one matrices $\mathbf{x}\mathbf{x}^T$, with $\mathbf{x}\in\mathbb{R}^n_+$, i.e.,

$$\mathcal{C}^* \,=\, \mathrm{conv}\,\{\,\mathbf{x}\mathbf{x}^T \,:\, \mathbf{x}\in\mathbb{R}^n_+\,\}. \tag{2.8}$$

Theorem 2.1 ([8])**.** *Let* $\mathbf{y}$ *be as in (2.6) and let* $\mathcal{C}_d \subset \mathcal{S}^n$ *be the closed convex cone*

$$\mathcal{C}_d \,:=\, \{\, \mathbf{A} \in \mathcal{S}^n \;:\; \mathbf{M}_d(f_{\mathbf{A}}\,\mathbf{y}) \,\succeq\, 0\,\}, \qquad d = 0, 1, \ldots \tag{2.9}$$

Then $\mathcal{C}_0 \supset \mathcal{C}_1 \cdots \supset \mathcal{C}_d \cdots \supset \mathcal{C}^*$ *and* $\mathcal{C} = \displaystyle\bigcap_{d=0}^{\infty} \mathcal{C}_d$.

The proof is a direct consequence of [8, Theorem 3.3] with $\mathbf{K} = \mathbb{R}^n_+$ and $f = f_{\mathbf{A}}$. Since $f_{\mathbf{A}}$ is homogeneous, alternatively one may use the probability measure ν uniformly supported on the n-dimensional simplex $\mathbf{K} = \{\mathbf{x} \in \mathbb{R}^n_+ : \sum_i x_i \leq 1\}$ and invoke [8, Theorem 3.2].

Observe that in view of the definition (2.2) of the localizing matrix, the entries of the matrix $\mathbf{M}_d(f_{\mathbf{A}}\,\mathbf{y})$ are linear in $\mathbf{A}$. Therefore, each convex cone $\mathcal{C}_d \subset \mathcal{S}^n$ is a spectrahedron in $\mathbb{R}^{n(n+1)/2}$ defined solely in terms of the entries (a_{ij}) of $\mathbf{A} \in \mathcal{S}^n$, and the hierarchy of spectrahedra $(\mathcal{C}_d)$, $d \in \mathbb{N}$, provides a nested sequence of outer approximations of $\mathcal{C}$. Also, testing whether a given matrix $\mathbf{A} \in \mathcal{S}^n$ belongs to $\mathcal{C}_d$ is an eigenvalue problem as one has to check whether the smallest eigenvalue of $\mathbf{M}_d(f_{\mathbf{A}}, \mathbf{y})$ is nonnegative. Therefore, instead of using standard packages for Linear Matrix Inequalities, one may use powerful specialized softwares for eigenvalues.

We next describe an inner approximation of the convex cone $\mathcal{C}^*$ via the hierarchy of convex cones $(\mathcal{C}^*_d)$, $d \in \mathbb{N}$, where each $\mathcal{C}^*_d$ is the dual cone of $\mathcal{C}_d$ in Theorem 2.1.

Recall that $\Sigma[\mathbf{x}]_d$ is the space of polynomials that are sums of squares of polynomials of degree at most d. A matrix $\mathbf{A} \in \mathcal{S}^n$ is also identified with a vector $\mathbf{a} \in \mathbb{R}^{n(n+1)/2}$ in the obvious way, and conversely, with any vector $\mathbf{a} \in \mathbb{R}^{n(n+1)/2}$ is associated a matrix $\mathbf{A} \in \mathcal{S}^n$. For instance, with $n = 2$,

$$\mathbf{A} \,=\, \left[\begin{array}{cc} a & b \\ b & c \end{array}\right] \quad \leftrightarrow \quad \mathbf{a} \,=\, \left[\begin{array}{c} a \\ 2b \\ c \end{array}\right]. \tag{2.10}$$

So we will not distinguish between a convex cone in $\mathbb{R}^{n(n+1)/2}$ and the corresponding cone in $\mathcal{S}^n$.

Theorem 2.2. *Let* $\mathcal{C}_d \subset \mathcal{S}^n$ *be the convex cone defined in (2.9). Then*

$$\mathcal{C}^*_d = \mathrm{cl}\,\left\{ (\langle\,\mathbf{X}, \mathbf{M}_d(x_i x_j\,\mathbf{y})\,\rangle\,)_{1\leq i\leq j\leq n} \;:\; \mathbf{X} \in \mathcal{S}^{s(d)}_+ \right\}. \tag{2.11}$$

Equivalently:

$$\begin{aligned} \mathcal{C}^*_d \quad &= \quad \mathrm{cl}\left\{ \int_{\mathbb{R}^n_+} \mathbf{x}\mathbf{x}^T \,\underbrace{\sigma(\mathbf{x})\,d\mu(\mathbf{x})}_{d\mu_\sigma(\mathbf{x})} \;:\; \sigma \in \Sigma[\mathbf{x}]_d \right\} \\ &= \quad \mathrm{cl}\,\left\{\, \mathbf{M}^2_1(\sigma\,\mathbf{y}) \;:\; \sigma \in \Sigma[\mathbf{x}]_d \,\right\}, \end{aligned} \tag{2.12}$$

with $\mathbf{M}^2_1(\sigma\,\mathbf{y})$ *as in (2.5).*

Proof. Let

$$\Delta_d \,:=\, \left\{ (\langle\,\mathbf{X}, \mathbf{M}_d(x_i x_j\,\mathbf{y})\,\rangle\,)_{1\leq i\leq j\leq n} \;:\; \mathbf{X} \in \mathcal{S}^{s(d)}_+ \right\},$$

so that

$$\begin{aligned}\Delta_d^* &= \left\{\mathbf{a}\in\mathbb{R}^{n(n+1)/2}\,:\,\sum_{1\le i\le j\le n} a_{ij}\,\langle\mathbf{X},\mathbf{M}_d(x_ix_j\,\mathbf{y}\rangle\ge 0\quad\forall\,\mathbf{X}\in\mathcal{S}_+^{s(d)}\right\},\\ &= \left\{\mathbf{a}\in\mathbb{R}^{n(n+1)/2}\,:\,\left\langle\mathbf{X},\mathbf{M}_d\left((\sum_{1\le i\le j\le n} a_{ij}x_ix_j)\,\mathbf{y}\right)\right\rangle\ge 0\quad\forall\,\mathbf{X}\in\mathcal{S}_+^{s(d)}\right\},\\ &= \{\mathbf{A}\in\mathcal{S}^n\,:\,\langle\mathbf{X},\mathbf{M}_d(f_{\mathbf{A}}\,\mathbf{y})\rangle\ge 0\quad\forall\,\mathbf{X}\in\mathcal{S}_+^{s(d)}\,\}\quad[\text{with }\mathbf{A},\mathbf{a}\text{ as in (2.10)}]\\ &= \{\mathbf{A}\in\mathcal{S}^n\,:\,\mathbf{M}_d(f_{\mathbf{A}}\,\mathbf{y})\succeq 0\,\}\,=\,\mathcal{C}_d.\end{aligned}$$

And so we obtain the desired result $\mathcal{C}_d^* = (\Delta_d^*)^* = \mathrm{cl}\,(\Delta_d)$. Next, writing the singular decomposition of $\mathbf{X}$ as $\sum_{k=0}^s \mathbf{q}_k\,\mathbf{q}_k^T$ for some $s\in\mathbb{N}$ and some vectors $(\mathbf{q}_k)\subset\mathbb{R}^{s(d)}$, one obtains that for every $1\le i\le j\le n$,

$$\begin{aligned}\langle\,\mathbf{X},\mathbf{M}_d(x_ix_j\,\mathbf{y})\,\rangle &= \sum_{k=0}^s\langle\,\mathbf{q}_k\mathbf{q}_k^T,\mathbf{M}_d(x_ix_j\,\mathbf{y})\,\rangle\,=\,\sum_{k=0}^s\langle\,\mathbf{q}_k,\mathbf{M}_d(x_ix_j\,\mathbf{y})\mathbf{q}_k\,\rangle\\ &= \sum_{k=0}^s\int x_ix_j\,q_k(\mathbf{x})^2\,d\mu(\mathbf{x})\quad[\text{by (2.4)}]\\ &= \int x_ix_j\,\underbrace{\sigma(\mathbf{x})\,d\mu(\mathbf{x})}_{d\mu_\sigma(\mathbf{x})},\end{aligned}$$

where $\sigma(\mathbf{x})=\sum_{k=0}^s q_k(\mathbf{x})^2\in\Sigma[\mathbf{x}]_d$, and $\mu_\sigma(B)=\int_B\sigma\,d\mu$ for all Borel sets B. □

So Theorem 2.2 states that $\mathcal{C}_d^*$ is the closure of the convex cone generated by second-order moments of measures $d\mu_\sigma=\sigma d\mu$, absolutely continuous with respect to μ (hence with support on $\mathbb{R}_+^n$) and with density being a s.o.s. polynomial σ of degree at most $2d$. Of course we immediately have:

Corollary 2.3. *Let $\mathcal{C}_d^*$, $d\in\mathbb{N}$, be as in (2.12). Then $\mathcal{C}_d^*\subset\mathcal{C}_{d+1}^*$ for all $d\in\mathbb{N}$, and*

$$\mathcal{C}^*\,=\,\mathrm{cl}\,\bigcup_{d=0}^\infty\mathcal{C}_d^*.$$

Proof. As $\mathcal{C}_d^*\subset\mathcal{C}_{d+1}^*$ for all $d\in\mathbb{N}$, the result follows from

$$\mathcal{C}^*\,=\,\left(\bigcap_{d=0}^\infty\mathcal{C}_d\right)^*\,=\,\mathrm{cl}\,\left(\mathrm{conv}\,\bigcup_{d=0}^\infty\mathcal{C}_d^*\right)\,=\,\mathrm{cl}\,\bigcup_{d=0}^\infty\mathcal{C}_d^*.$$

□

In other words, $\mathcal{C}_d^*$ approximates $\mathcal{C}^*=\mathrm{conv}\,\{\mathbf{x}\mathbf{x}^T:\mathbf{x}\in\mathbb{R}_+^n\}$ (i.e., the convex hull of second-order moments of Dirac measures with support in $\mathbb{R}_+^n$) from inside by second-order moments of measures $\mu_\sigma\ll\mu$ whose density is a s.o.s. polynomial σ of degree at most $2d$, and better and better approximations are obtained by letting d increase.

Example 1. For instance, with $n=2$, and $\mathbf{A}=\begin{bmatrix}a & b\\ b & c\end{bmatrix}$, it is known that

$$\mathbf{A}\text{ is copositive if and only if }a,c\ge 0\text{ and }b+\sqrt{ac}\ge 0.$$

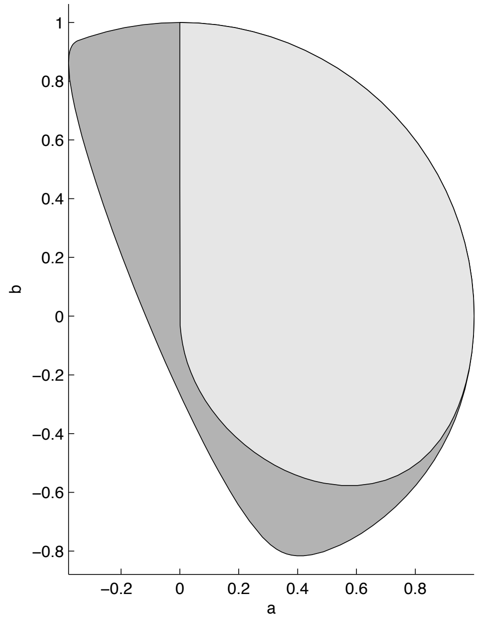

FIGURE 1. $n = 2$: Projection on the (a, b)-plane of $\mathcal{C}$ versus $\mathcal{C}_1$, both intersected with the unit ball

With $f_{\mathbf{A}}(\mathbf{x}) := ax_1^2 + 2bx_1x_2 + cx_2^2$ and $d = 1$, the condition $\mathbf{M}_d(f_{\mathbf{A}}\,\mathbf{y}) \succeq 0$ which reads

$$\left[\begin{array}{ccc} a+b+c & 3a+2b+c & a+2b+3c \\ 3a+2b+c & 12a+6b+2c & 3a+4b+3c \\ a+2b+3c & 3a+4b+3c & 2a+6b+12c \end{array}\right] \succeq 0,$$

defines the convex cone $\mathcal{C}_1 \subset \mathbb{R}^3$. It is a connected component of the basic semi-algebraic set $\{(a, b, c) : \det(\mathbf{M}_1(f_{\mathbf{A}}\,\mathbf{y})) \geq 0\}$, that is, elements (a, b, c) such that:

$$3a^3 + 15a^2b + 29a^2c + 16ab^2 + 50abc + 29ac^2 + 4b^3 + 16b^2c + 15bc^2 + 3c^3 \;\geq\; 0.$$

Figure 1 below displays the projection on the (a, b)-plane of the sets $\mathcal{C}_1$ and $\mathcal{C}$ intersected with the unit ball.

2.3. **An alternative representation of the cone $\mathcal{C}_d^*$.** From its definition (2.11) in Theorem 2.2, the cone $\mathcal{C}_d^* \subset \mathcal{S}^n$ is defined through the matrix variable $\mathbf{X} \in \mathcal{S}^{s(d)}$ which lives in a (lifted) space of dimension $s(d)(s(d) + 1)/2$ and with the linear matrix inequality (LMI) constraint $\mathbf{X} \succeq 0$ of size $s(d)$ (whereas $\mathcal{C}_d$ does not need any lifting).

We next provide another explicit description on how $\mathcal{C}_d^*$ can be generated with no LMI constraint and with only $s(d)$ variables, but of course this characterization is not well suited for optimization purposes.

Since every $g \in \Sigma[\mathbf{x}]_d$ can be written $\sum_\ell g_\ell^2$ for finitely many polynomials $(g_\ell) \subset \mathbb{R}[\mathbf{x}]_d$, the convex cone $\Sigma[\mathbf{x}]_d$ of s.o.s. polynomials can be written

$$\Sigma[\mathbf{x}]_d \;=\; \mathrm{conv}\,\{g^2 \;:\; g \in \mathbb{R}[\mathbf{x}]_d\,\}.$$

Next, for $g\in\mathbb{R}[\mathbf{x}]_d$, with vector of coefficients $\mathbf{g}=(g_\alpha)\in\mathbb{R}^{s(d)}$, let $\mathbf{g}^{(2)}=(g^{(2)}_\alpha)\in\mathbb{R}^{s(2d)}$ be the vector of coefficients of g^2, that is,

$$g(\mathbf{x})=\sum_{\alpha\in\mathbb{N}^n_d} g_\alpha\,\mathbf{x}^\alpha \quad\rightarrow\quad g(\mathbf{x})^2\,=\,\sum_{\alpha\in\mathbb{N}^n_{2d}} g^{(2)}_\alpha\,\mathbf{x}^\alpha.$$

Notice that for each $\alpha\in\mathbb{N}^n_{2d}$, $g^{(2)}_\alpha$ is quadratic in $\mathbf{g}$. For instance, with $n=2$ and $d=1$, $g(\mathbf{x})=g_{00}+g_{10}x_{10}+g_{01}x_{01}$ with $\mathbf{g}=(g_{00},\,g_{10},g_{01})^T\in\mathbb{R}^{s(1)}$, and so

$$\mathbf{g}^{(2)}\,=\,(g_{00}^2,\,2g_{00}g_{10},\,2g_{00}g_{01},\,g_{10}^2,\,2g_{10}g_{01},\,g_{02}^2)^T\in\mathbb{R}^{s(2)}.$$

Next, for every $1\le i\le j\le n$, let $\mathbf{G}_d=(G_{ij})\in\mathcal{S}^n$ be defined by:

$$G_{ij}\,:=\sum_{\alpha\in\mathbb{N}^n_{2d}}\frac{g^{(2)}_\alpha}{(\alpha_i+1)!(\alpha_j+1)!}\prod_{k\neq i,j}\frac{1}{\alpha_k!},\qquad 1\le i\le j\le n. \tag{2.13}$$

We can now describe $\mathcal{C}^*_d$.

Corollary 2.4. *Let $\mathbf{G}_d\in\mathcal{S}^n$ be as in (2.13). Then:*

$$\mathcal{C}^*_d\,=\,\mathrm{cl}\,\left(\mathrm{conv}\,\{\mathbf{G}_d\,:\,\mathbf{g}\in\mathbb{R}^{s(d)}\,\}\right). \tag{2.14}$$

The characterization (2.14) of $\mathcal{C}^*_d$ should be compared with the characterization $\mathrm{conv}\,\{\mathbf{x}\mathbf{x}^T\,:\,\mathbf{x}\in\mathbb{R}^n_+\}$ of $\mathcal{C}$.

Example 2. *With $n=2$ and $d=1$, $\mathbf{G}_1$ reads:*

$$\left[\begin{array}{cc} 12g_{00}^2+8g_{10}(g_{00}+g_{01})+24g_{00}g_{01}+g_{10}^2+6g_{01}^2 & 24g_{00}(g_{00}+g_{10}+g_{01})+4(g_{10}^2+g_{01}^2)+12g_{10}g_{01}\\ 24g_{00}(g_{00}+g_{10}+g_{01})+4(g_{10}^2+g_{01}^2)+12g_{10}g_{01} & 12g_{00}^2+24g_{00}g_{10}+8g_{01}(g_{00}+g_{10})+6g_{10}^2+g_{01}^2\end{array}\right]$$

2.4. **$\mathcal{K}$-copositive and $\mathcal{K}$-completely positive matrices.** Let $\mathcal{K}\subset\mathbb{R}^n$ be a closed convex cone and let $\mathcal{C}_\mathcal{K}$ be the convex cone of $\mathcal{K}$-copositive matrices, i.e., matrices $\mathbf{A}\in\mathcal{S}^n$ such that $\mathbf{x}^T\mathbf{A}\mathbf{x}\ge0$ on $\mathcal{K}$. Its dual cone $\mathcal{C}^*_\mathcal{K}\subset\mathcal{S}^n$ is the cone of $\mathcal{K}$-completely positive matrices.

Then one may define a hierarchy of convex cones $(\mathcal{C}_{\mathcal{K}d})$ and $(\mathcal{C}^*_{\mathcal{K}d})$, $d\in\mathbb{N}$, formally exactly as in Theorem 2.1 and Theorem 2.2, but now $\mathbf{y}$ is the moment sequence of a finite Borel measure μ with $\mathrm{supp}\,\mu=\mathcal{K}$ (instead of $\mathrm{supp}\,\mu=\mathbb{R}^n_+$ in (2.6)), i.e., $\mathbf{y}=(y_\alpha)$, $\alpha\in\mathbb{N}^n$, with:

$$y_\alpha\,:=\int_\mathcal{K}\mathbf{x}^\alpha\,d\mu,\qquad\forall\alpha\in\mathbb{N}^n\quad\text{(and where }\mathrm{supp}\,\mu=\mathcal{K}). \tag{2.15}$$

And so with $\mathbf{y}$ as in (2.15) Theorem 2.1 and 2.2, as well as Corollary 2.3, are still valid. (In (2.12 replace $\int_{\mathbb{R}^n_+}$ with $\int_\mathcal{K}$). Therefore,

$$\mathcal{C}_\mathcal{K}\,=\,\bigcap_{d=0}^\infty\mathcal{C}_{\mathcal{K}d}\quad\text{and}\quad\mathcal{C}^*_\mathcal{K}\,=\,\mathrm{cl}\,\bigcup_{d=0}^\infty\mathcal{C}^*_{\mathcal{K}d}.$$

But of course, for practical implementation, one need to know the sequence $\mathbf{y}=(y_\alpha)$, which was easy when $\mathcal{K}=\mathbb{R}^n_+$. For instance, if $\mathcal{K}$ is a polyhedral cone, by homogeneity of $f_\mathbf{A}$, one may equivalently consider a compact base of $\mathcal{K}$ (which is a polytope $\mathcal{K}'$), and take for μ the Lebesgue measure on $\mathcal{K}'$. Then all moments of μ can be calculated exactly. The same argument works for every convex cone $\mathcal{K}$ for which one may compute all moments of a finite Borel measure μ whose support is a compact base of $\mathcal{K}$.

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