Copositive optimization — recent developments and applications

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Abstract

Due to its versatility, copositive optimization receives increasing interest in the Operational Research community, and is a rapidly expanding and fertile field of research. It is a special case of conic optimization, which consists of minimizing a linear function over a cone subject to linear constraints. The diversity of copositive formulations in different domains of optimization is impressive, since problem classes both in the continuous and discrete world, as well as both deterministic and stochastic models are covered. Copositivity appears in local and global optimality conditions for quadratic optimization, but can also yield tighter bounds for NP-hard combinatorial optimization problems. Here some of the recent success stories are told, along with principles, algorithms and applications.

1. Introduction

1.1. Motivation, notation and basic ideas

Copositive optimization (or copositive programming, coined in [19]) is a special case of conic optimization, which consists of minimizing a linear function over a (convex) cone subject to additional (inhomogeneous) linear (inequality or equality) constraints. This problem class has a close connection to that of quadratic optimization, which represents the simplest class of hard problems in continuous optimization [102] – to minimize a (possibly indefinite) quadratic form over a poly-

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hedron given in standard form:

$$\min\left\{\mathbf{x}^\top Q\mathbf{x} : A\mathbf{x} = \mathbf{b}\,,\ \mathbf{x}\in\mathbb{R}^n_+\right\}\,. \tag{1}$$

Here we denote by bold-faced letters vectors in n-dimensional Euclidean space $\mathbb{R}^n$, the positive orthant therein by $\mathbb{R}^n_+$ (we write $\mathbf{a}\geq\mathbf{b}$ for $\mathbf{a}-\mathbf{b}\in\mathbb{R}^n_+$), and by $^\top$ transposition. I_n is the $n\times n$ identity matrix (sometimes with subscript suppressed if the order of I_n is clear from the context), $\mathbf{o}$ and O stand for zero vectors, and matrices, respectively, of appropriate orders. For two integers m and n with $m\leq n$ we abbreviate $[m\!:\!n]$ for the integer interval $\{m, m+1,\dots,n\}$.

The basic *lifting* idea (see, e.g. [92]) is to linearize the quadratic form

$$\mathbf{x}^\top Q\mathbf{x} = \operatorname{trace}(\mathbf{x}^\top Q\mathbf{x}) = \operatorname{trace}(Q\mathbf{x}\mathbf{x}^\top) = \langle Q, \mathbf{x}\mathbf{x}^\top\rangle$$

by introducing the new symmetric matrix variable $X=\mathbf{x}\mathbf{x}^\top$ and Frobenius duality $\langle X,Y\rangle = \operatorname{trace}(XY)$. If $A\mathbf{x}\in\mathbb{R}^m_+$ for all $\mathbf{x}\in\mathbb{R}^n_+$ and $\mathbf{b}\in\mathbb{R}^m_+$, then the linear constraints in (1) can be squared, to arrive in a similar way at linear constraints of the form $\langle A_i, X\rangle = b_i^2$, where $A_i=\mathbf{a}_i\mathbf{a}_i^\top$ and $\mathbf{a}_i^\top$ is the i-th row of A.

Now the set of all these $X=\mathbf{x}\mathbf{x}^\top$ generated by feasible $\mathbf{x}$ is non-convex since rank $(\mathbf{x}\mathbf{x}^\top)=1$. The convex hull

$$\mathcal{C} = \operatorname{conv}\left\{\mathbf{x}\mathbf{x}^\top : \mathbf{x}\in\mathbb{R}^n_+\right\}\,,$$

results in a convex matrix cone called the cone of *completely positive matrices* since [71]; for a text see [7]. Note that a similar construction dropping nonnegativity constraints leads to

$$\mathcal{P} = \operatorname{conv}\left\{\mathbf{x}\mathbf{x}^\top : \mathbf{x}\in\mathbb{R}^n\right\}\,,$$

the cone of positive-semidefinite matrices, the basic set in *Semidefinite Optimization (SDP)*, wherefrom above lifting idea was borrowed.

1.2. Terminology, duality and attainability

Duality theory for conic optimization problems requires the dual cone $\mathcal{C}^*$ of $\mathcal{C}$ w.r.t. the Frobenius inner product which is

$$\mathcal{C}^* = \{S \text{ a symmetric } n\times n \text{ matrix} : \langle S, X\rangle \geq 0 \text{ for all } X\in\mathcal{C}\}\,.$$

Here it can easily be shown that $\mathcal{C}^*$ coincides with the cone of *copositive matrices*, namely

$$\mathcal{C}^* = \left\{S \text{ a symmetric } n\times n \text{ matrix} : \mathbf{x}^\top S\mathbf{x}\geq 0 \text{ for all } \mathbf{x}\in\mathbb{R}^n_+\right\}\,.$$

This observation justifies terminology of our problem class. The term was coined by T.S. Motzkin (the usually cited source [106] however provides no evidence of this) who called a matrix S copositive (apparently abbreviating "*co*nditionally *positive*-semidefinite"), if S generates a quadratic form $\mathbf{x}^\top S\mathbf{x}$ taking no negative values over the positive orthant. More generally, let $\Gamma \subseteq \mathbb{R}^n$ be a closed convex cone and consider the class

$$\mathcal{C}_\Gamma^* = \left\{ S \text{ a symmetric } n \times n \text{ matrix} : \mathbf{x}^\top S\mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \Gamma \right\}$$

of all Γ-*copositive matrices*. This is the dual cone of

$$\mathcal{C}_\Gamma = \text{conv } \left\{ \mathbf{x}\mathbf{x}^\top : \mathbf{x} \in \Gamma \right\} .$$

The first accounts on copositive optimization can be found in [116, 19], where a copositive representation of a subclass of particular interest is established, namely for *Standard Quadratic Optimization Problems (StQPs)*. Here the feasible polyhedron is the standard simplex $\Delta = \left\{ \mathbf{x} \in \mathbb{R}^n_+ : \mathbf{e}^\top \mathbf{x} = 1 \right\}$, where $\mathbf{e} = [1, \ldots, 1]^\top \in \mathbb{R}^n$: this subclass is also NP-hard (there can be up to $\sim 2^n/(1.25\sqrt{n})$ local non-global solutions [14]). Now, with $E = \mathbf{e}\mathbf{e}^\top$ the $n \times n$ all-ones matrix, we have

$$\min \left\{ \mathbf{x}^\top Q\mathbf{x} : \mathbf{x} \in \Delta \right\} = \min \left\{ \langle Q, X \rangle : \langle E, X \rangle = 1 \, , \; X \in \mathcal{C} \right\} . \tag{2}$$

Note that the problem on the right-hand side is convex, so there are no more local, non-global solutions. In addition, the objective function is now linear, and there is just one linear equality constraint. The complexity has been completely pushed into the feasibility condition $X \in \mathcal{C}$, which also shows that there are indeed convex minimization problems which cannot be solved easily: while the most prominent conic optimization problems, namely SDPs, second-order cone optimization, and linear optimization problems (LPs), can be solved to arbitrary accuracy in polynomial time, copositive problems are NP-hard. The dual of problem (2) over $\mathcal{C}$ is then

$$\max \left\{ y \in \mathbb{R} : S = Q - yE \in \mathcal{C}^* \right\} , \tag{3}$$

a linear objective in just one variable y with the innocent-looking feasibility constraint $S \in \mathcal{C}^*$. This shows that checking membership of $\mathcal{C}^*$ is NP-hard, which has been observed already by [102]. More generally, a typical primal-dual pair in copositive optimization is of the following form:

$$\begin{aligned} & \inf \left\{ \langle C, X \rangle : \langle A_i, X \rangle = b_i \, , i \in [1:m] \, , \; X \in \mathcal{C} \right\} \\ \geq \; & \sup \left\{ \mathbf{b}^\top \mathbf{y} : \mathbf{y} \in \mathbb{R}^m \, , \, S = C - \textstyle\sum_i y_i A_i \in \mathcal{C}^* \right\} . \end{aligned}$$

The inequality above is just standard weak duality, but observe we have to use inf and sup since – as in general conic optimization – there may be problems with attainability of either or both problems above, and likewise there could be a (finite or infinite) positive duality gap without any further conditions like strict feasibility (*Slater's condition*). For the above representation of StQPs, this is not the case:

$$\min\{\langle Q,X\rangle : \langle E,X\rangle = 1\,,\ X\in\mathcal{C}\} = \max\{y : S = Q - yE \in \mathcal{C}^*\}\ .$$

But for a similar class arising in many applications, the *Multi-Standard Quadratic Optimization Problems* [25], dual attainability is not guaranteed while the duality gap is zero – an intermediate form between weak and strong duality [117]. A complete picture of possible attainability/duality gap constellations in primal-dual pairs of copositive optimization problems is provided in [26], which also lists some elementary algebraic properties and counterexamples illustrating the difference between the semidefinite cone $\mathcal{P}$ and the copositive/completely positive cone $\mathcal{C}^*/\mathcal{C}$. This is important for many copositivity detection procedures, and as we saw in (3), the feasibility constraint incorporates most of the hardness in copositive optimization.

1.3. Surveys, reviews, entries, book chapters

Copositive optimization receives increasing interest in the Operational Research community, and is a rapidly expanding and fertile field of research. While the time may not yet be ripe for writing up the final standard text book in this domain, several authors nonetheless bravely took the challenge of providing an overview, thereby aiming at a rapidly moving target. A recent survey on copositive optimization is offered by [57], while [77] and [74] provide reviews on copositivity with less emphasis on optimization. Bomze [16] and Busygin [37] provided entries in the most recent edition of the Encyclopedia of Optimization. Recent book chapters with some character of a survey on copositivity from an optimization viewpoint are [17, Section 1.4] and [34]. Finally, [26] offers a rough literature review by clustering a considerable part of copositivity-related publications.

1.4. Organization of this paper

We start in Section 2 by demonstrating the diversity of copositive formulations in different domains of optimization: continuous and discrete, deterministic and stochastic. Section 3 briefly sketches the ideas of approximation hierarchies, a field with many contacts to (semi-)algebraic geometry and positive polynomials, therefore closely related to the Positivstellensatz [120, 118, 114], an extension of Hilbert's famous Nullstellensatz. Also some complexity issues are discussed here. We turn to the core of Operational Research in discussing the role of copositivity for local and global optimality conditions in Section 4. In the world of quadratic optimization, it turns out that checking global optimality requires an effort which differs from that of checking local optimality only by a factor smaller than the number of constraints. This may be somewhat surprising at first thought. On the other hand, elementary geometric intuition also suggests that the gap between global and local optimization opens more widely when curvature of the objective is no longer constant. In Section 5, we give a short account on some algorithmic approaches to checking copositivity, and to solve copositive optimization problems. Finally, in Section 6, some success stories are reported: how to obtain tractable yet tight bounds for NP-complete combinatorial problems like the Maximum-Clique problem, how to find the best known asymptotic bound for crossing numbers, and, in the continuous domain, how to construct tight convex underestimators by means of copositive optimization, or Lyapunov functions for switched dynamical systems in optimal control.

2. Copositive reformulations of NP-hard problems

2.1. The standard quadratic case

This case was already addressed above as a motivating (and historically first) example for copositive reformulation, see [116] and [19]. The Maximum-Clique Problem provides a thoroughly studied example of application, see Section 6.3. So consider the StQP

$$\alpha_Q = \min\left\{\mathbf{x}^\top Q\mathbf{x} : \mathbf{x} \in \Delta\right\} , \tag{4}$$

and its copositive formulation

$$\alpha_Q = \min\left\{\langle Q, X\rangle : \langle E, X\rangle = 1\,,\ X \in \mathcal{C}\right\} .$$

Not only the optimal values are equal, we also know there is always a rank-one solution X^* to the latter problem over $\mathcal{C}$, which encodes an optimal solution $\mathbf{x}^*$ to the StQP (4) by way of $X^* = \mathbf{x}^*(\mathbf{x}^*)^\top$. However, if there are multiple optimal solutions to the former (or the latter), we only know that any optimal solution $\overline{X}$ (which may be returned by an – ideal – copositive optimization procedure) is a convex combination of rank-one solutions of the type X^* above. Therefore a rounding procedure is required to retrieve the solution of the StQP in general, unless the above addressed procedure 'automatically' delivers a rank-one solution. In any case, a strength of this approach is that the optimal value is found, or at least a valid bound thereof if an approximation as in Section 3.1 is used.

2.2. The fractional quadratic case

In engineering applications, one frequently encounters friction and resonance problems which can be cast into fractional quadratic optimization problems of the type

$$\psi = \min\left\{ f(\mathbf{x}) = \frac{\mathbf{x}^\top C\mathbf{x} + 2\mathbf{c}^\top \mathbf{x} + \gamma}{\mathbf{x}^\top B\mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + \beta} : A\mathbf{x} = \mathbf{a}\,,\ \mathbf{x} \in \mathbb{R}^n_+ \right\}\,, \tag{5}$$

where $B \in \mathcal{P}$ and C is a symmetric $n \times n$ matrix, $\{\mathbf{b}, \mathbf{c}\} \subset \mathbb{R}^n$, A is an $m \times n$ matrix, and $\mathbf{a} \in \mathbb{R}^m$. This NP-hard problem also arises when studying the repair of inconsistent linear systems, for details see [1]. Now define the symmetric $(n+1) \times (n+1)$ matrices

$$\overline{A} = \left[\begin{array}{cc} \mathbf{a}^\top\mathbf{a} & -\mathbf{a}^\top A \\ -A^\top\mathbf{a} & A^\top A \end{array}\right]\,, \quad \overline{B} = \left[\begin{array}{cc} \beta & \mathbf{b}^\top \\ \mathbf{b} & B \end{array}\right]\,, \quad \overline{C} = \left[\begin{array}{cc} \gamma & \mathbf{c}^\top \\ \mathbf{c} & C \end{array}\right]\,,$$

and assume that the problem in (5) is well defined; to be more precise, we assume that

$$\left.\begin{array}{l} \left\{\mathbf{x} \in \mathbb{R}^n_+ : A\mathbf{x} = \mathbf{a}\right\} \neq \emptyset \text{ and} \\ A\mathbf{y} \neq \mathbf{o} \text{ for all } \mathbf{y} \in \mathbb{R}^n_+ \setminus \{\mathbf{o}\} \text{ and} \\ \mathbf{z}^\top\overline{B}\mathbf{z} > 0 \text{ if } \overline{A}\mathbf{z} = \mathbf{o}\,,\ \mathbf{z} \in \mathbb{R}^{n+1}_+ \setminus \{\mathbf{o}\}\,. \end{array}\right\} \tag{6}$$

Then [113] (for the special case $\left\{\mathbf{x} \in \mathbb{R}^n_+ : A\mathbf{x} = \mathbf{a}\right\} = \Delta$) and [1] showed under (6) that (5) can be written as the completely positive problem:

$$\psi = \min\left\{\langle\overline{C}, X\rangle : \langle\overline{B}, X\rangle = 1\,,\ \langle\overline{A}, X\rangle = 0\,,\ X \in \mathcal{C}\right\}\,.$$

Again, a rank-one optimal solution to the latter problem encodes an optimal solution to (5) as in the StQP case.

2.3. Mixed-binary QPs: Burer's reformulation and beyond

Burer showed in [33] a result generalizing that of Section 2.1: take any (possibly empty) subset $B \subseteq [1\!:\!n]$ and abbreviate by $\{0,1\}^B_n$ the set of all vectors $\mathbf{x} \in \mathbb{R}^n$ which have binary coordinates $x_j \in \{0,1\}$ for $j \in B$. Then under mild conditions any mixed-binary quadratic optimization problem

$$p^* = \min\left\{\mathbf{x}^\top Q\mathbf{x} + 2\mathbf{c}^\top\mathbf{x} : A\mathbf{x} = \mathbf{b}\,,\ \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n\right\}$$

can be represented as a copositive optimization problem, with $\mathcal{A}$ a linear map from $\mathcal{C}$ to $\mathbb{R}^d$:

$$p^* = \min \left\{ \langle \widehat{Q}, \widehat{X} \rangle : \mathcal{A}(\widehat{X}) = \widehat{\mathbf{b}} \, , \, \widehat{X} \in \mathcal{C} \right\}$$

where $\widehat{X}$ and $\widehat{Q}$ are $(n+1) \times (n+1)$ matrices, and the size of $(\mathcal{A}, \widehat{\mathbf{b}})$ is polynomial in the size of $(A, \mathbf{b})$. Very recently, inspired by [22], Burer generalized in [34] the sign constraints $\mathbf{x} \in \mathbb{R}^n_+$ above in an elegant way to arbitrary cone constraints $\mathbf{x} \in \Gamma$, where Γ is a closed, convex cone, i.e., studying the (non-convex) *quadratic cone-constrained problem*

$$p^* = \min \left\{ \mathbf{x}^\top Q \mathbf{x} + 2\mathbf{c}^\top \mathbf{x} : A\mathbf{x} = \mathbf{b} \, , \; \mathbf{x} \in \Gamma \right\} . \tag{7}$$

Again, the dimension of the problem is increased by one, by enriching the vector $\mathbf{x} \in \Gamma$ with an additional nonnegative number $\zeta > 0$, i.e., passing from the cone $\Gamma \subseteq \mathbb{R}^n$ to the cone $\widehat{\Gamma} = \mathbb{R}_+ \times \Gamma$, and considering $\mathcal{C}_{\widehat{\Gamma}} = \operatorname{conv} \left\{ \mathbf{z}\mathbf{z}^\top : \mathbf{z} \in \widehat{\Gamma} \right\}$, the dual cone of the cone $\mathcal{C}^*_{\widehat{\Gamma}}$ of all $\widehat{\Gamma}$-copositive $(n+1) \times (n+1)$ matrices. Fixing the additional variable ζ to unity, we arrive at the feasible set

$$\mathcal{R} = \left\{ Y = \begin{bmatrix} 1 & \mathbf{x}^\top \\ \mathbf{x} & X \end{bmatrix} \in \mathcal{C}_{\widehat{\Gamma}} : A\mathbf{x} = \mathbf{b} \, , \; (AXA^\top)_{ii} = b_i^2 \text{ for all } i \right\} ,$$

and problem (7) is equivalent, in the way described in the previous sections, to the (generalized) completely positive problem

$$p^* = \min \left\{ \langle \widehat{Q}, Y \rangle : Y \in \mathcal{R} \right\} \quad \text{with} \quad \widehat{Q} = \begin{bmatrix} 0 & \mathbf{c}^\top \\ \mathbf{c} & Q \end{bmatrix} . \tag{8}$$

One may wonder how binarity constraints $x_j \in \{0, 1\}$ enter the scene now. But observe that any such constraint can be written as a quadratic one, namely $x_j^2 - x_j = 0$. This quadratic constraint can be captured by imposing the constraint $X_{jj} - x_j = 0$ on $Y \in \mathcal{R}$, provided that $0 \le x_j \le 1$ whenever $A\mathbf{x} = \mathbf{b}$ and $\mathbf{x} \in \Gamma$ (this would be one of the mild conditions mentioned at the beginning of this section; for a comment on these in context of relaxations see [80]). In a similar way, we also can incorporate complementarity constraints of the form $x_i x_j = 0$ by imposing $X_{ij} = 0$. More generally, assume, e.g., that all variables occurring in the quadratic function $\mathbf{x}^\top F \mathbf{x} + 2\mathbf{f}^\top \mathbf{x}$ are bounded on the feasible set $\{\mathbf{x} \in \Gamma : A\mathbf{x} = \mathbf{b}\}$ of (7) and put

$$\gamma = \min \left\{ \mathbf{x}^\top F \mathbf{x} + 2\mathbf{f}^\top \mathbf{x} : A\mathbf{x} = \mathbf{b} \, , \; \mathbf{x} \in \Gamma \right\} .$$

Consider the quadratically constrained problem

$$p_q^* = \min \left\{ \mathbf{x}^\top Q \mathbf{x} + 2\mathbf{c}^\top \mathbf{x} : A\mathbf{x} = \mathbf{b} \, , \; \mathbf{x}^\top F \mathbf{x} + 2\mathbf{f}^\top \mathbf{x} = \gamma \, , \mathbf{x} \in \Gamma \right\} . \tag{9}$$

Then

$$p_q^* = \min \left\{ \langle \widehat{Q}, Y \rangle : \langle \widehat{F}, Y \rangle = \gamma \,, \; Y \in \mathcal{R} \right\} \quad \text{with} \quad \widehat{F} = \begin{bmatrix} 0 & \mathbf{f}^\top \\ \mathbf{f} & F \end{bmatrix} \tag{10}$$

is equivalent to (9) is the above described sense. See [59] for a recent parallel development using the copositive cone $\mathcal{C}^*$, independent from [34].

2.4. Copositive formulation of robust optimization with uncertain objective

In a similar domain [105] provide a completely positive formulation. They consider a mixed-binary linear optimization problem with stochastic objective function of which only the first two moments are known. In the usual robust optimization approach, they ask to maximize the expected optimal value of this stochastic optimization model; see also [66]. Problems of this kind have widespread applications, e.g., for network reliability questions. To be more precise, the following problem is treated:

$$z^* = \sup \left\{ \mathbb{E} \left[\max \left\{ \tilde{\mathbf{c}}^\top \mathbf{x} : A\mathbf{x} = \mathbf{b} \,, \; \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n \right\} \right] : \tilde{\mathbf{c}} \sim (\boldsymbol{\mu}, \Sigma)_+ \right\} \,, \tag{11}$$

where the symbol $\tilde{\mathbf{c}} \sim (\boldsymbol{\mu}, \Sigma)_+$ means that the supremum is taken over all probability distributions of the random vector $\tilde{\mathbf{c}} \in \mathbb{R}^n$ which have support in the positive orthant $\mathbb{R}^n_+$ and fixed first and second moments: $\mathbb{E}(\tilde{\mathbf{c}}) = \boldsymbol{\mu}$ and $\mathbb{E}\left[\tilde{\mathbf{c}}\tilde{\mathbf{c}}^\top\right] = \Sigma$. Only those moment combinations $(\boldsymbol{\mu}, \Sigma)$ are considered which allow for such distributions (which implies, e.g., that $\boldsymbol{\mu} \in \mathbb{R}^n_+$). In general, it is difficult to test this condition, but it is satisfied if $\begin{bmatrix} 1 & \boldsymbol{\mu}^\top \\ \boldsymbol{\mu} & \Sigma \end{bmatrix}$ is in the interior of $\mathcal{C}$. Further assumptions are as in the previous section ($A\mathbf{x} = \mathbf{b}$ and $\mathbf{x} \in \mathbb{R}^n_+$ imply $0 \le x_j \le 1$ for all $j \in B$), along with boundedness of the inner feasible set $\left\{ \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n : A\mathbf{x} = \mathbf{b} \right\}$, which ensures that the expected value is bounded and thus z^* as defined in (11) is finite. Then it is shown in [105] that

$$\begin{aligned} z^* \; = \; \max \{ &\operatorname{trace}(Z) \colon \; A\mathbf{x} = \mathbf{b}, \; (AXA^\top)_{ii} = b_i^2 \text{ for all } i \in [1\!:\!n] \text{ and} \\ &X_{jj} = x_j \text{ for all } j \in B, \; T_{(\boldsymbol{\mu},\Sigma)}(\mathbf{x}, X, Z) \in \mathcal{C} \; \} \,, \end{aligned} \tag{12}$$

where

$$T_{(\boldsymbol{\mu},\Sigma)}(\mathbf{x}, X, Z) = \begin{bmatrix} 1 & \boldsymbol{\mu}^\top & \mathbf{x}^\top \\ \boldsymbol{\mu} & \Sigma & Z^\top \\ \mathbf{x} & Z & X \end{bmatrix}$$

is a symmetric $(2n+1) \times (2n+1)$ matrix (note that the $n \times n$ matrix Z need not be symmetric). This recent development possibly opens new bridges from the

SDP approaches of *Cross Moment Models (CMM)* and chance constraining via *generalized Chebyshev bounds* à la [124] to copositive optimization and its higher-order relaxations. For this reason, the authors of [105] suggest to call problem (12) *Completely Positive Cross Moment Model (CPCMM)*. They also show an approximate equivalence result similar to those in the previous sections: for any optimal solution $(\mathbf{x}^*, X^*, Z^*)$ of (12), they construct a sequence $\tilde{\mathbf{c}}_k$ of random vectors (with discrete distributions on $\mathbb{R}^n_+$) such that $\mathbb{E}\tilde{\mathbf{c}}_k \to \boldsymbol{\mu}$ and $\mathbb{E}\left[\tilde{\mathbf{c}}_k\tilde{\mathbf{c}}_k^\top\right] \to \Sigma$ as $k \to \infty$ as well as

$$\mathbb{E}\left[\max\left\{\tilde{\mathbf{c}}_k^\top \mathbf{x} : A\mathbf{x} = \mathbf{b}\,,\ \mathbf{x} \in \mathbb{R}^n_+ \cap \{0,1\}^B_n\right\}\right] \to z^* = \mathrm{trace}(Z^*)\,.$$

Evidently, (12) can be extended to describe situations where the first two moments $(\boldsymbol{\mu}, \Sigma)$ are not known exactly but only some bounds on them.

3. Approximation hierarchies and complexity issues

3.1. Approximation and tractable bounds

We already convinced ourselves that the cones $\mathcal{C}^*$ and $\mathcal{C}$ cannot be tractable unless NP equals P. Hence for large problems we need a tractable approximation cone, say $\mathcal{K}$, which is closely related to, say $\mathcal{C}$, e.g., in the sense that $\mathcal{C} \subset \mathcal{K}$ but $\mathcal{K}\setminus\mathcal{C}$ is not too large. Since we know that $\mathcal{C} \subset \mathcal{P}$, this implies at least $\mathcal{K} \subset \mathcal{P} = \mathcal{P}^*$. By duality, we know

$$\mathcal{C} \subset \mathcal{K} \subset \mathcal{P} \subset \mathcal{K}^* \subset \mathcal{C}^*\,.$$

The general principle to obtain tractable bounds, then, would use above inclusion to arrive at

$$\begin{aligned} & \inf\left\{\langle C, X\rangle : \langle A_i, X\rangle = b_i\,,\ i \in [1\!:\!m]\,,\ X \in \mathcal{C}\right\} \\ \geq\ & \inf\left\{\langle C, X\rangle : \langle A_i, X\rangle = b_i\,,\ i \in [1\!:\!m]\,,\ X \in \mathcal{K}\right\}\,, \end{aligned}$$

and, on the dual side,

$$\begin{aligned} & \sup\left\{\mathbf{b}^\top\mathbf{y} : \mathbf{y} \in \mathbb{R}^m\,,\ S = C - \textstyle\sum_i y_i A_i \in \mathcal{C}^*\right\} \\ \geq\ & \sup\left\{\mathbf{b}^\top\mathbf{y} : \mathbf{y} \in \mathbb{R}^m\,,\ S = C - \textstyle\sum_i y_i A_i \in \mathcal{K}^*\right\}\,. \end{aligned}$$

Note that strong duality can either apply to the dual pair with $\mathcal{C}$ and $\mathcal{C}^*$, or to $\mathcal{K}$ and $\mathcal{K}^*$, or to both.

The simplest choice for such a tractable cone of course is $\mathcal{P}$ itself. A tighter option is $\mathcal{P} \cap \mathcal{N}$ where

$$\mathcal{N} = \{N \text{ a symmetric } n \times n \text{ matrix } : N_{ij} \geq 0 \text{ for all } \{i,j\} \subseteq [1\!:\!n]\}$$

denotes the cone of nonnegative matrices. In a larger part of the literature, matrices in $\mathcal{P}\cap\mathcal{N}$ are called *doubly nonnegative.* It is immediate that $(\mathcal{P}\cap\mathcal{N})^* = \mathcal{P}^*+\mathcal{N}^* = \mathcal{P}+\mathcal{N}$, so that we arrive

$$\mathcal{C} \subseteq \mathcal{P}\cap\mathcal{N} \subset \mathcal{P}+\mathcal{N} \subseteq \mathcal{C}^*\,,$$

which also shows that $\mathcal{C}$ never can be self-dual, unlike $\mathcal{P} = \mathcal{P}^*$ and $\mathcal{N} = \mathcal{N}^*$. Hence, we unfortunately cannot apply the whole theory of symmetric cones from conic optimization. For $n \geq 5$, already Alfred Horn noted that the left-most and the right-most inclusion above are strict [71, 51].

Copositive approximation hierarchies [108, 86, 18, 109, 67, 126, 53] start with the *zero-order approximation* $\mathcal{K}^{(0)} = \mathcal{P}+\mathcal{N}$ whose dual cone is the above discussed $\mathcal{P}\cap\mathcal{N}$, and consist of an increasing sequence $\mathcal{K}^{(r)}$ of cones satisfying $\mathrm{cl}\left(\cup_{r\geq 0}\mathcal{K}^{(r)}\right) = \mathcal{C}^*$. For instance, a higher-order approximation due to [108] uses squaring the variables to get rid of sign constraints: $S\in\mathcal{C}^*$ if and only if $\mathbf{y}^\top S\mathbf{y}\geq 0$ for all $\mathbf{y}$ such that $y_i = x_i^2$ for some $\mathbf{x}\in\mathbb{R}^n$, and this is guaranteed if the n-variable polynomial of degree $2(r+2)$ in $\mathbf{x}$,

$$p_S^{(r)}(\mathbf{x}) = (\sum x_i^2)^r \mathbf{y}^\top S\mathbf{y} = (\sum x_i^2)^r \sum_{j,k} S_{jk}x_j^2x_k^2$$

is nonnegative for all $\mathbf{x}\in\mathbb{R}^n$. But this holds in particular, if

(a) $p_S^{(r)}$ has no negative coefficients; or if

(b) $p_S^{(r)}$ is a sum-of-squares (s.o.s.):

$$p_S^{(r)}(\mathbf{x}) = \sum_i [f_i(\mathbf{x})]^2\,, \quad f_i \text{ some polynomials.}$$

This gives the approximation cones

$$\mathcal{C}^{(r)} = \{S \text{ a symmetric } n\times n \text{ matrix } : S \text{ satisfies (a)}\}\,,$$

and

$$\mathcal{K}^{(r)} = \{S \text{ a symmetric } n\times n \text{ matrix } : S \text{ satisfies (b)}\}\,.$$

While $\mathcal{C}^{(r)}$ can be described by linear constraints on the entries of S, leading to LP formulations, the cones $\mathcal{K}^{(r)}$ are described by *linear matrix inequalities (LMI's)*, leading to SDP formulations. Basically, the monomials $\mathbf{x}^{\mathbf{m}} = \prod_i x_i^{m_i}$ occurring in $p_S^{(r)}$ are replaced with new variables $z_{\mathbf{m}}$ and condition (b) above is rephrased as a positive-semidefiniteness condition on a suitable quadratic form $\mathbf{z}^\top M\mathbf{z}$ in these variables. However, both cones $\mathcal{C}^{(r)}$ and $\mathcal{K}^{(r)}$ are computationally intractable for large r, as they generate problems on matrices M of order $\mathcal{O}(n^{r+1}\times n^{r+1})$; for details, see, e.g. [18].

3.2. Complexity issues for the StQP case

General complexity issues in this context are discussed in [49, 45]. For the sake of conciseness, we concentrate here on the StQP case which forms an instance of NP-hard problems which admit a *polynomial-time approximation scheme (PTAS)*. This is in sharp contrast to the case of box-constrained QPs [6] and may be intuitively explained by the fact that, unlike the hypercube, the volume of the standard simplex decreases exponentially fast in n as dimension n increases. Also, this poses no contradiction to the well-known inapproximability results [72] for the clique number $\omega(G)$, since the StQP formulation (30) in Section 6.3 below provides the inverse value $\frac{1}{\omega(G)}$.

For simplicity of exposition we will employ the LP hierarchy $\mathcal{C}^{(r)}$. Remember

$$\begin{aligned}
\alpha_Q &= \min\left\{\mathbf{x}^\top Q\mathbf{x} : \mathbf{x}\in\Delta\right\}\\
&= \min\left\{\langle Q, X\rangle : \langle E, X\rangle = 1\,,\ X\in\mathcal{C}\right\}\\
&= \max\left\{y\in\mathbb{R} : Q - yE \in \mathcal{C}^*\right\}\\
&\geq \max\left\{y\in\mathbb{R} : Q - yE \in \mathcal{C}^{(r)}\right\} =: \alpha_Q^{\mathcal{C}^{(r)}}\,.
\end{aligned}$$

Denote by $\mathbb{N}_0 = \mathbb{N}\cup\{0\}$ the set of all nonnegative integers and consider the following rational grid approximation of Δ with $\binom{n+r+1}{r+1} = \mathcal{O}\left(n^{r+1}\right)$ points:

$$\Delta(r) = \left\{\mathbf{z}\in\Delta : (r+2)\mathbf{z}\in\mathbb{N}_0^n\right\}\,.$$

Then one can show [18]

$$\alpha_Q^{\mathcal{C}^{(r)}} = \tfrac{r+2}{r+1}\min\left\{\mathbf{x}^\top Q\mathbf{x} - \mathbf{q}_r^\top\mathbf{x} : \mathbf{x}\in\Delta(r)\right\}\,,$$

with $\mathbf{q}_r = \frac{1}{r+2}\,\mathrm{diag}\,(Q)$. The naïve counterpart to the above simply optimizes over the finite grid, which of course provides an upper bound:

$$\alpha_Q^{\Delta(r)} = \min\left\{\mathbf{x}^\top Q\mathbf{x} : \mathbf{x}\in\Delta(r)\right\} \geq \alpha_Q \geq \alpha_Q^{\mathcal{C}^{(r)}}\,.$$

This way, we enclose the desired value α_Q from below and above. The approximation error bound can be estimated as follows [18]: put $\beta_Q = \max\left\{\mathbf{x}^\top Q\mathbf{x} : \mathbf{x}\in\Delta\right\}$. Then $\beta_Q - \alpha_Q$ is the span of Q over Δ, and we have

$$\begin{aligned}
0 &\leq \alpha_Q - \alpha_Q^{\mathcal{C}^{(r)}} \leq \tfrac{1}{r+1}\left(\beta_Q - \alpha_Q\right) \quad \text{and}\\
0 &\leq \alpha_Q^{\Delta(r)} - \alpha_Q \leq \tfrac{1}{r+2}\left(\beta_Q - \alpha_Q\right).
\end{aligned}$$

As a consequence, we now deduce that StQPs belong to the PTAS class. Indeed, for arbitrarily small $\mu > 0$, StQP allows for polynomial-time implementable μ-approximation. Again, for $\mu = \frac{1}{r+1}$, we need an effort of $|\Delta(r)| = \mathcal{O}\left(n^{r+1}\right)$. There are better constants than the span $\beta_Q - \alpha_Q$ [126].

4. Role of copositivity in second-order optimality conditions

4.1. Local optimality conditions in QPs

For ease of presentation we mostly concentrate on quadratic optimization problems in this section. However, some of the results can be generalized to smooth problems with nonlinear constraints, see Remark 4.2 below. So let us consider here a QP in slightly different form than above:

$$\min\left\{f(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^\top Q\mathbf{x} + \mathbf{c}^\top\mathbf{x} : \mathbf{x} \in M\right\}, \tag{13}$$

with Q a symmetric $n \times n$ matrix, $M = \{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} \le \mathbf{b}\}$, A an $m \times n$ matrix and $\mathbf{b} \in \mathbb{R}^m$. Expressed in terms of the *Lagrangian function* $L(\mathbf{x};\mathbf{u}) = f(\mathbf{x}) + \mathbf{u}^\top(A\mathbf{x} - \mathbf{b})$ where $\mathbf{u} \in \mathbb{R}^m_+$ contains the Lagrange multipliers for the inequality constraints, the *first-order optimality (KKT) conditions* read

$$\nabla_{\mathbf{x}} L(\overline{\mathbf{x}};\mathbf{u}) = \mathbf{o} \quad \text{and} \quad \mathbf{u}^\top(A\overline{\mathbf{x}} - \mathbf{b}) = 0\,, \quad (\overline{\mathbf{x}},\mathbf{u}) \in M \times \mathbb{R}^m_+\,. \tag{14}$$

To remove inefficient solution candidates, we have to employ *second-order optimality conditions*, using constant curvature: both the objective and the Lagrangian functions have the Hessian matrix $\nabla^2_{\mathbf{x}} L(\mathbf{x};\mathbf{u}) = \nabla^2 f(\mathbf{x}) = Q$ for all $(\mathbf{x},\mathbf{u}) \in M \times \mathbb{R}^m_+$. Denote the set of *active constraints* at $\overline{\mathbf{x}}$ by

$$I(\overline{\mathbf{x}}) = \left\{i \in [1\!:\!m] : \mathbf{a}_i^\top \overline{\mathbf{x}} = b_i\right\},$$

with $\mathbf{a}_i^\top$ the i-th row of A. The local view of M from $\overline{\mathbf{x}}$ is captured by the tangent cone, which due to linearity of constraints coincides with the cone of feasible directions at $\overline{\mathbf{x}}$,

$$\Gamma(\overline{\mathbf{x}}) = \mathbb{R}_+(M - \overline{\mathbf{x}}) = \left\{\mathbf{v} \in \mathbb{R}^n : \mathbf{a}_i^\top \mathbf{v} \le 0 \text{ for all } i \in I(\overline{\mathbf{x}})\right\}. \tag{15}$$

Note that (14) implies the weak first-order ascent condition $\mathbf{v}^\top \nabla f(\overline{\mathbf{x}}) \ge 0$ for all $\mathbf{v} \in \Gamma(\overline{\mathbf{x}})$. Moreover, even strict first-order ascent directions may be negative curvature directions as

$$f(\overline{\mathbf{x}} + t\mathbf{v}) - f(\overline{\mathbf{x}}) = t\left[\mathbf{v}^\top \nabla f(\overline{\mathbf{x}}) + \tfrac{t}{2}\,\mathbf{v}^\top Q\mathbf{v}\right] > 0\,, \tag{16}$$

if $t > 0$ is small enough and $\mathbf{v}^\top \nabla f(\overline{\mathbf{x}}) > 0$, even if $\mathbf{v}^\top Q\mathbf{v} < 0$. Thus we concentrate on the *reduced tangent cone*

$$\Gamma_{\mathrm{red}}(\overline{\mathbf{x}}) = \left\{\mathbf{v} \in \Gamma(\overline{\mathbf{x}}) : \mathbf{v}^\top \nabla f(\overline{\mathbf{x}}) = 0\right\} \tag{17}$$

and stipulate $\mathbf{v}^\top Q\mathbf{v} \geq 0$ for all $\mathbf{v} \in \Gamma_{\text{red}}(\overline{\mathbf{x}})$ only, i.e., that Q be $\Gamma_{\text{red}}(\overline{\mathbf{x}})$-copositive. We arrive at a first formulation: under (14), $\overline{\mathbf{x}}$ is a local solution to (13) if and only if Q is $\Gamma_{\text{red}}(\overline{\mathbf{x}})$-copositive. Else, any $\mathbf{v} \in \Gamma_{\text{red}}(\overline{\mathbf{x}})$ with $\mathbf{v}^\top Q\mathbf{v} < 0$ is a strictly improving feasible direction. Below, a more complete version of this characterization and also a historical account of it will be provided.

Because $\Gamma_{\text{red}}(\overline{\mathbf{x}})$ is a polyhedral cone, it is possible, although tedious, to check $\Gamma_{\text{red}}(\overline{\mathbf{x}})$-copositivity by finite procedures, see Section 5.1 below. Here it may suffice to notice that this condition is clearly satisfied if Q is positive-semidefinite, an aspect of the well-known result that in convex problems, KKT points are (global) solutions. Generally, it is NP-hard to check copositivity even if the cone $\Gamma_{\text{red}}(\overline{\mathbf{x}})$ is very simple. This is not surprising in view of the result that checking local optimality of KKT points is NP-hard [102]. See [58] for a thorough discussion of more general copositivity notions and their properties.

Remark 4.1. *Given a vector of Lagrange multipliers $\mathbf{u} \in \mathbb{R}^m_+$ for a KKT point $\overline{\mathbf{x}}$, one can define the cone*

$$\Gamma^{\triangle}_{\mathbf{u}} = \{\mathbf{v} \in \Gamma(\overline{\mathbf{x}}) : \mathbf{a}_i^\top \mathbf{v} = 0 \text{ for all } i \text{ with } u_i > 0\}\,. \tag{18}$$

While it is easy to see that $\Gamma^{\triangle}_{\mathbf{u}}(\overline{\mathbf{x}}) = \Gamma_{\text{red}}(\overline{\mathbf{x}})$ for any set of Lagrange multipliers $\mathbf{u}$, *some authors, e.g. [93, 63, 89], use (18) to define the reduced tangent cone, from which it may not immediately be evident that this cone does not depend on the particular choice of* $\mathbf{u}$. *The alternative, preferable definition (17) occurs, e.g., in [40, 27].*

4.2. Strict local optimality versus strict complementarity, also beyond QPs

Recall that $\overline{\mathbf{x}}$ is said to satisfy the *strict complementarity* condition in (14) if all Lagrange multipliers at active constraints are strictly positive: $u_i > 0$ for all $i \in I(\overline{\mathbf{x}})$. By contrast, $\overline{\mathbf{x}}$ is said to be a *strict local solution* to (13) if there is a neighbourhood U of $\overline{\mathbf{x}}$ in M such that

$$f(\mathbf{x}) > f(\overline{\mathbf{x}}) \quad \text{for all } \mathbf{x} \in U \setminus \{\overline{\mathbf{x}}\}\ .$$

We are now ready to present a more detailed version of the second-order conditions for (strict) local optimality of KKT points in (13). To this end, recall that a symmetric matrix Q is called *strictly* Γ*-copositive*, if $\mathbf{v}^\top Q\mathbf{v} > 0$ holds for all $\mathbf{v} \in \Gamma \setminus \{\mathbf{o}\}$. Most of the results in the next theorem can be traced back to [93, 89] (with the drawbacks indicated in Remark 4.1 above). Then [40] corrected an error in [93]. In turn, [27] closed a lacuna in the argumentation of [40], and finally established the result in a much more general, infinite-dimensional setting. Here we follow the presentation in [14].

$$\left.\begin{array}{l}\overline{\mathbf{x}} \text{ is a local solution to (13) if and only if (14) holds and} \\ Q \text{ is } \Gamma_{\text{red}}(\overline{\mathbf{x}})\text{-copositive,}\end{array}\right\} \qquad (19)$$

and

$$\left.\begin{array}{l}\overline{\mathbf{x}} \text{ is a strict local solution to (13) if and only if (14) holds and} \\ Q \text{ is strictly } \Gamma_{\text{red}}(\overline{\mathbf{x}})\text{-copositive.}\end{array}\right\} \qquad (20)$$

Moreover, if $\overline{\mathbf{x}}$ satisfies strict complementarity, then the cone $\Gamma_{\text{red}}(\overline{\mathbf{x}})$ becomes a linear subspace, namely $\Gamma_{\text{red}}(\overline{\mathbf{x}}) = \{\mathbf{a}_i : i \in I(\overline{\mathbf{x}})\}^{\perp}$. In this case, choose an $n \times r$ matrix U whose columns span $\Gamma_{\text{red}}(\overline{\mathbf{x}})$. Then

$$\left.\begin{array}{l}\overline{\mathbf{x}} \text{ is a local solution to (13) if and only if (14) holds and} \\ \overline{Q} = U^{\top} Q U \text{ is positive-semidefinite,}\end{array}\right\} \qquad (21)$$

and

$$\left.\begin{array}{l}\overline{\mathbf{x}} \text{ is a strict local solution to (13) if and only if (14) holds and} \\ \overline{Q} = U^{\top} Q U \text{ is positive-definite.}\end{array}\right\} \qquad (22)$$

From a practical point of view, we see that the characterizations (21) and (22) are much more convenient because checking definiteness of a smaller $r \times r$ matrix can be done in polynomial time whereas checking copositivity is NP-hard [102]. Contrasting with several other procedures (e.g., the simplex method for LPs), this difference in worst-case complexity is also reflected in the actual average case behaviour.

Similar conditions are employed, e.g., in [64] or, more recently, in [39]. Frequently, these conditions are divided in a necessary part (involving semidefiniteness) and a sufficient part (involving definiteness), which as shown above is not needed. Rather, this difference distinguishes the case of strict solutions from the case of nonstrict ones.

Remark 4.2. *The local optimality conditions (19) and (20) are formulated for QPs, but can be generalized quite easily to more general problems with nonquadratic* *objective and nonlinear constraints, at the cost of opening then a gap between necessary (copositivity) and sufficient (strict copositivity) conditions, and under the requirement of additional constraint qualifications for the necessary part, see, e.g.[63, p.81]. To summarize, under appropriate conditions one has the following rough picture:*

$$\textit{strict copositivity} \Rightarrow \textit{strict local solution} \Rightarrow \textit{local solution} \Rightarrow \textit{copositivity}\,, \tag{23}$$

while for QPs, relation (23) can be sharpened as follows:

$$\textit{strict copositivity} \Leftrightarrow \textit{strict local solution} \Rightarrow \textit{local solution} \Leftrightarrow \textit{copositivity}\,. \tag{24}$$

Another consequence of (22) is that a local solution satisfying the strict complementarity condition is necessarily strict, if $\overline{Q}$ is nonsingular (then all four conditions in (24) are equivalent). Unfortunately, this kind of argument does not carry over to (23), because from nonsingularity of a copositive matrix Q one cannot infer strict copositivity [14]; this reflects the fact that there are non-strict local solutions which do satisfy strict complementarity.

4.3. Global optimality conditions in QPs via copositivity

The number of local, non-global solutions to (13) may be exponential in the number of variables and/or constraints [17]. Therefore it is reasonable to formulate conditions which characterize global rather than local optimality. To this end, denote by $\mathbf{s} = \mathbf{b} - A\overline{\mathbf{x}}$ the vector of slack variables, and by $J(\overline{\mathbf{x}}) = [0\!:\!m] \setminus I(\overline{\mathbf{x}})$. To have a consistent notation, we can also view as $J(\overline{\mathbf{x}})$ as the set of inactive constraints if we add an auxiliary inactive constraint of the form $0 < 1$ by enriching $(A, \mathbf{b})$ with a 0-th row to

$$\bar{A} = \begin{bmatrix} \mathbf{a}_0^\top \\ \\ A \\ \\ \end{bmatrix} = \begin{bmatrix} \mathbf{o}^\top \\ \mathbf{a}_1^\top \\ \vdots \\ \mathbf{a}_m^\top \end{bmatrix}, \quad \bar{\mathbf{b}} = \begin{bmatrix} b_0 \\ \\ \mathbf{b} \\ \\ \end{bmatrix} = \begin{bmatrix} 1 \\ b_1 \\ \vdots \\ b_m \end{bmatrix},$$

and put $\bar{\mathbf{s}} = \bar{\mathbf{b}} - \bar{A}\bar{\mathbf{x}} \geq \mathbf{o}$. Then $J(\overline{\mathbf{x}}) = \{i \in [0\!:\!m] : \bar{s}_i > 0\}$. The 0-th slack and the corresponding constraint will be needed for dealing with unbounded feasible directions. However, if $\mathbf{v}$ is a bounded feasible direction, then there is an $i \in J(\overline{\mathbf{x}}) \setminus \{0\}$ such that $\mathbf{a}_i^\top(\overline{\mathbf{x}} + t\mathbf{v}) > b_i$ for some $t > 0$, and the *maximal feasible stepsize* in direction of $\mathbf{v}$

$$\bar{t}_{\mathbf{v}} = \min\left\{\frac{\bar{s}_i}{\bar{\mathbf{a}}_i^\top \mathbf{v}} : i \in J(\overline{\mathbf{x}})\,,\ \bar{\mathbf{a}}_i^\top \mathbf{v} > 0\right\}$$

is finite.

Note that feasibility of a direction $\mathbf{v} \in \mathbb{R}^n$ is fully characterized by the property $\mathbf{a}_i^\top \mathbf{v} \leq 0$ for all i with $s_i = 0$, i.e., for all i in the complement of $J(\overline{\mathbf{x}})$. If in addition, $\mathbf{a}_i^\top \mathbf{v} \leq 0$ for all $i \in J(\overline{\mathbf{x}})$, i.e., $A\mathbf{v} \leq \mathbf{o}$ but $\mathbf{v} \neq \mathbf{o}$, then we have an unbounded feasible direction with $\bar{t}_\mathbf{v} = +\infty$ by the usual default rules, consistent with the property that $\overline{\mathbf{x}} + t\mathbf{v} \in M$ for all $t > 0$ in this case. In the opposite case where $\bar{t}_\mathbf{v} = \frac{s_i}{\mathbf{a}_i^\top \mathbf{v}} < +\infty$, we have $i \neq 0$, and the i-th constraint is the first inactive constraint which becomes active when travelling from $\overline{\mathbf{x}}$ along the ray given by $\mathbf{v}$: then $\overline{\mathbf{x}} + \bar{t}_\mathbf{v}\mathbf{v} \in M$, but $\overline{\mathbf{x}} + t\mathbf{v} \notin M$ for all $t > \bar{t}_\mathbf{v}$.

By consequence, the feasible polyhedron M is decomposed into a union of polytopes $M_i(\overline{\mathbf{x}}) = \{\mathbf{x} = \overline{\mathbf{x}} + t\mathbf{v} \in M : 0 \leq t \leq \bar{t}_\mathbf{v}\}$ for $i \in J(\overline{\mathbf{x}}) \setminus \{0\}$, and $M_0(\overline{\mathbf{x}}) = \{\mathbf{x} \in \mathbb{R}^n : A\mathbf{x} \leq A\overline{\mathbf{x}}\}$, the (possibly trivial, but otherwise) unbounded polyhedral part of M.

To be more precise, we need the $(m+1) \times n$-matrices $D_i = \bar{\mathbf{s}}\,\mathbf{a}_i^\top - \bar{s}_i \bar{A}$ to define the polyhedral cones

$$\Gamma_i = \{\mathbf{v} \in \mathbb{R}^n : D_i\mathbf{v} \geq \mathbf{o}\}\ , \quad i \in J(\overline{\mathbf{x}})\,. \tag{25}$$

Then $\bigcup_{i \in J(\overline{\mathbf{x}})} \Gamma_i = \Gamma(\overline{\mathbf{x}})$ from (15), and $M_i(\overline{\mathbf{x}}) = M \cap (\Gamma_i + \overline{\mathbf{x}})$ contains all points $\mathbf{x} \in M$ where $i \in J(\overline{\mathbf{x}})$ denotes the first inactive constraint which becomes active when travelling along direction $\mathbf{x} - \overline{\mathbf{x}}$ starting from $\overline{\mathbf{x}}$ (as mentioned above, the case $i = 0$ captures unbounded feasible directions).

After these preparations dealing with the feasible set only, we turn to the objective function. With the gradient $\nabla f(\bar{\mathbf{x}}) = Q\bar{\mathbf{x}} + \mathbf{c}$, we construct rank-two updates of Q:

$$Q_i = \mathbf{a}_i\, \nabla f(\bar{\mathbf{x}})^\top + \nabla f(\bar{\mathbf{x}})\, \mathbf{a}_i^\top + \bar{s}_i Q\,, \quad i \in J(\overline{\mathbf{x}})\,. \tag{26}$$

Now the *extremal increment* $\theta_{\overline{\mathbf{x}}}(\mathbf{v}) = f(\overline{\mathbf{x}} + \bar{t}_\mathbf{v}\mathbf{v}) - f(\overline{\mathbf{x}})$ satisfies for $\mathbf{v}^\top Q\mathbf{v} < 0$, see (16),

$$f(\overline{\mathbf{x}} + t\mathbf{v}) - f(\overline{\mathbf{x}}) \geq 0 \quad \text{ for all } \mathbf{x} = \overline{\mathbf{x}} + t\mathbf{v} \in M\ \text{, i.e., } t \in [0, \bar{t}_\mathbf{v}]\,,$$

if and only if $\theta_{\overline{\mathbf{x}}}(\mathbf{v}) \geq 0$. For $\mathbf{v} \in \Gamma_i$, the condition $\theta_{\overline{\mathbf{x}}}(\mathbf{v}) \geq 0$ can be expressed as $\mathbf{v}^\top Q_i\mathbf{v} \geq 0$. Hence we have that

$$\left.\begin{array}{l} \overline{\mathbf{x}} \text{ is a global solution to (13) if and only if (14) holds and} \\ Q_i \text{ are } \Gamma_i\text{-copositive} \quad \text{ for all } i \in J(\bar{\mathbf{x}})\,. \end{array}\right\} \tag{27}$$

Else, if $\mathbf{v}^\top Q_i \mathbf{v} < 0$ and $D_i \mathbf{v} \geq \mathbf{o}$ for some $i \in J(\overline{\mathbf{x}}) \setminus \{0\}$, then $\mathbf{a}_i^\top \mathbf{v} > 0$ and

$$\widetilde{\mathbf{x}} = \bar{\mathbf{x}} + \bar{t}_{\mathbf{v}} \mathbf{v} \quad \text{is an improving feasible point,}$$

whereas $\mathbf{v}^\top Q_0 \mathbf{v} < 0$ for some $\mathbf{v}$ with $D_0 \mathbf{v} \geq \mathbf{o}$ if and only if (13) is unbounded.

Note that the result above also applies to QPs for which the Frank/Wolfe-Theorem is non-trivial, i.e., where the objective function f is bounded from below over an unbounded polyhedron M (see [107] and [117] for a recent survey and extensions of the Frank/Wolfe-Theorem).

Comparing conditions (19) and (27), we see that the effort of checking local versus global optimality is not that different: at most m copositivity checks instead of merely one. Condition (27) was first established for the concave case using ε-subdifferential calculus [44], and later on for the indefinite case in an article [9] which appeared in print before [44]. For a recent discussion of local optimality under the perspective of ε-subdifferential calculus, also beyond QPs, see [24].

5. Algorithmic copositivity detection and copositive optimization

5.1. Copositivity detection: recursive procedures

Explicit copositivity criteria in low dimensions ($n = 2$ or $n = 3$) are well-known since long, see, e.g. [68]. To proceed towards recursive copositivity detection, one may decompose

$$Q = \begin{bmatrix} \alpha & \mathbf{b}^\top \\ \mathbf{a} & C \end{bmatrix}$$

where $\mathbf{b} \in \mathbb{R}^{n-1}$ and C is an $(n-1) \times (n-1)$ matrix.

For any vector $\mathbf{v} \in \mathbb{R}^m$, let $\Gamma_{\mathbf{v}} = \left\{ \mathbf{z} \in \mathbb{R}^m_+ : \mathbf{v}^\top \mathbf{z} \geq 0 \right\}$. Then Q is $\mathbb{R}^n_+$-copositive if and only if [8] either

$$\left.\begin{array}{l} \alpha = 0\,,\ \mathbf{b} \in \mathbb{R}^{n-1}_+\,,\ \text{and } C \text{ is copositive; or} \\ \alpha > 0\,,\ C \text{ is } \Gamma_{\mathbf{b}}\text{-copositive, and } C - \frac{1}{\alpha}\mathbf{b}\mathbf{b}^\top \text{ is } \Gamma_{-\mathbf{b}}\text{-copositive.} \end{array}\right\} \tag{28}$$

This result gives rise to a branch-and-bound procedure for copositivity detection: the root of the problem tree is labeled by the data $(Q, \mathbb{R}^n_+)$; branching (and sometimes pruning) consists of checking signs of the first row of Q: if $\alpha < 0$, we can prune the tree at this node with the information that Q is not copositive, likewise for $\alpha = 0$ and $\mathbf{b} \notin \mathbb{R}^{n-1}_+$. If $\alpha \geq 0$ and $\mathbf{b} \in \mathbb{R}^{n-1}_+$, we generate one successor node labeled by $(C, \mathbb{R}^{n-1}_+)$, i.e., we just drop the nonnegative row and column. If $\alpha > 0$ but $\mathbf{b} \notin \mathbb{R}^{n-1}_+$, the next generation consists of the two nodes labeled by $(C, \Gamma_{\mathbf{b}})$ and $(C - \frac{1}{\alpha}\mathbf{b}\mathbf{b}^\top, \Gamma_{-\mathbf{b}})$: we have reduced problem dimension by one, but added linear constraints. This is the reason why we have to keep track not only of the resulting matrices, but also of the polyhedral cones w.r.t. which we have to check copositivity. We prune at a node (Q, Γ) if $\Gamma = \{\mathbf{o}\}$ is trivial (or, more generally, one may check whether Γ is contained in the linear subspace spanned by eigenvectors to nonnegative eigenvalues of Q, if $\Gamma \neq \{\mathbf{o}\}$). The leaves in the problem tree are characterized by 1×1 matrices on $\pm\mathbb{R}_+$, so a simple sign check does the job here.

For continuing this branching, we thus need a generalization of above characterization via (28) for general Γ-copositivity if Γ is a polyhedral cone given by a finite set of linear inequalities. In general, there can be much more successor nodes than just two in the root, and the problem tree will be far from binary. To reduce the number of successors, one may employ also a one-step look ahead strategy as in strong branching [8]. A block variant of this strategy can be found in [11], which in turn renders as a corollary the following improvement upon [81, Theorem 4]; see also [15]:

Let Q be a symmetric $n \times n$ matrix with block structure

$$Q = \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix} \quad \text{and partition} \quad I_n = \begin{bmatrix} E & F \end{bmatrix} \text{ accordingly,}$$

where A is a symmetric positive-definite $k \times k$ matrix, and E is an $n \times k$ matrix. Define Q_A and Γ_A as the *Schur complement* and the corresponding cone by

$$Q_A = C - B^\top A^{-1} B \quad \text{and} \quad \Gamma_A = \{\mathbf{z} \in \mathbb{R}^{n-k} : (F - EA^{-1}B)\mathbf{z} \geq \mathbf{o}\}\,.$$

Then

(a) if Q is copositive, then Q_A is Γ_A-copositive;

(b) if Q_A is copositive, then Q is copositive.

Further, if $-A^{-1}B \geq O$, then $\mathbb{R}^{n-k}_+ \subseteq \Gamma_A$, so that (a) and (b) together imply the following criterion:

$$Q \text{ is copositive if and only if } Q_A \text{ is copositive.}$$

As a spinoff of this result one obtains a linear-time algorithm for copositivity detection of (block-)tridiagonal matrices [13], which has been extended to acyclic matrices in [76]. Earlier algorithmic attempts in a similar vein can be found, e.g., in [51, 41, 94, 123, 43].

5.2. Decomposition and adaptive approaches

By positive homogeneity, Q is copositive if and only if $\mathbf{x}^\top Q\mathbf{x} \geq 0$ for all $\mathbf{x} \in \Delta$. Similarly, suppose

$$\mathbb{R}^n_+ = \bigcup_{i\in I} \mathbb{R}_+\Delta_i$$

for nonempty Δ_i. Then Q is copositive if and only if $\mathbf{x}^\top Q\mathbf{x} \geq 0$ for all $\mathbf{x} \in \Delta_i$ and all $i \in I$. Now, if $\Delta_i = \operatorname{conv}(\mathbf{w}_1, \ldots, \mathbf{w}_k)$ is a polytope with $k \geq n$ known vertices collected in an $n \times k$ matrix $W_i = [\mathbf{w}_1, \ldots, \mathbf{w}_k]$, every $\mathbf{x} \in \Delta_i$ can be written in *barycentric coordinates:* $\mathbf{x} = W_i\mathbf{v}$ for some $\mathbf{v} \in \Delta \subset \mathbb{R}^k$, and $\mathbf{x}^\top Q\mathbf{x}$ has the *Bézier-Bernstein representation* $\mathbf{x}^\top Q\mathbf{x} = \mathbf{v}^\top Q_i\mathbf{v}$ with $Q_i = W_i^\top QW_i$. Therefore

$$\mathbf{x}^\top Q\mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \Delta_i \quad \text{if and only if} \quad Q_i \text{ is copositive.}$$

Unlike in the previous section, Q_i are $k \times k$ matrices with $k \geq n$, but some of them may more likely satisfy sufficient conditions for copositivity like those in the following section. The simplest one is of course $Q_i \in \mathcal{N}$. Again, we may employ branch-and-bound by discarding those Δ_i and subdivide others where such a sufficient criterion fails, until convergence or detection of a violating vector $\mathbf{v} \in \mathbb{R}^n_+$ with $\mathbf{v}^\top Q\mathbf{v} < 0$. This is the common idea of the papers [30], [31], and [20].

In [30], the authors use subsimplices Δ_i of Δ, the sufficient condition $Q_i \in \mathcal{N}$, and in case of failure bisect the longest edge of Δ_i corresponding to a negative entry. A violating vector is detected whenever a negative diagonal element of Q_i occurs (recall that these equal $\mathbf{v}_j^\top Q\mathbf{v}_j$ for some vertex $\mathbf{v}_j$ of Δ_i).

In [31], this strategy is refined with respect to selection of the subsimplex to be bisected, according to the objective function in the copositive optimization problem. This is the adaptive aspect which turns a copositivity check into a fully-fledged procedure to solve copositive optimization problems, and apparently the algorithm in [31] is hard to beat up to now, but see [126, 128]. Working on the dual cone $\mathcal{C}$, the recent paper [23] suggests a factorization heuristic for solving copositive optimization problems.

A different approach is presented in [20], which uses more intricate sufficient and necessary copositivity conditions, and also a more sophisticated choice of simplices $\Delta_i = \operatorname{conv}(\mathbf{w}_1, \ldots, \mathbf{w}_n)$, which need not be part of the standard simplex. The key idea there is to use a *difference-of-convex decomposition (d.c.d.)* of Q, i.e., to select $\{Q_+, Q_-\} \subset \mathcal{P}$ such that $Q = Q_+ - Q_-$. Suppose for simplicity that both Q_+ and Q_- are nonsingular, and rescale

$$\mathbf{v}_j^- = \frac{1}{\sqrt{\mathbf{w}_i^\top Q_-\mathbf{w}_i}}\mathbf{w}_j\,,\; j \in [1\!:\!n]\,.$$

If $\min_j (\mathbf{v}_j^-)^\top Q_+ (\mathbf{v}_j^-) < 1$, a violating vector in Δ_i is found; else the following convex QP over the rescaled subsimplex is solved:

$$\mu_i^- = \min \left\{ \mathbf{v}^\top Q_+ \mathbf{v} : \mathbf{v} \in \text{conv}\,(\mathbf{v}_1^-, \dots, \mathbf{v}_n^-) \right\} . \tag{29}$$

If $\mu_i^- \geq 1$, then Q is $(\mathbb{R}_+\Delta_i)$-copositive; else the solution to (29) is used for ω-subdivision of Δ_i and for branching.

5.3. Shortcuts and preprocessing

As already mentioned, a very simple sufficient condition for copositivity of Q is $Q \in \mathcal{N}$. Likewise, we know that Q is copositive if $Q \in \mathcal{P}$. Based upon the idea described above, [20] also provides a generalization of the latter: given a d.c.d. $Q = Q_+ - Q_-$, choose an $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{p} = Q_+\mathbf{x}$ has only positive entries (this can be done, e.g., by an LP $\max\left\{\mathbf{f}^\top\mathbf{x} : Q_+\mathbf{x} \geq \mathbf{e}\,,\, \mathbf{x} \in \mathbb{R}^n_+\right\}$).

$$\text{If} \quad (Q_-)_{ii}\,\mathbf{x}^\top Q_+\mathbf{x} \leq (Q_+\mathbf{x})_i^2 \quad \text{for all } i \in [1\!:\!n]\,, \quad \text{then} \quad Q \text{ is copositive.}$$

This criterion requires a d.c.d. of Q, which can be found by spectral decomposition and truncating negative/positive eigenvalues of Q to zero, to obtain Q_+/Q_-, respectively. This variant requires knowledge of the eigenpairs $(\lambda_i, \mathbf{u}_i)$ but then the next tests are almost for free. They partly go back to [73], see also [15] and [20]. For any vector $\mathbf{u} \in \mathbb{R}^n$ denote by $\mathbf{u}^+ = [u_i^+]_i \in \mathbb{R}^n_+$ and $\mathbf{u}^- = \mathbf{u}^+ - \mathbf{u} \in \mathbb{R}^n_+$. Suppose that $Q \notin \mathcal{P}$ and order the eigenvalues of Q such that $\lambda_1 \leq \cdots \leq \lambda_k < 0 \leq \lambda_{k+1} \leq \cdots \leq \lambda_n$.

- If $\lambda_1 < -\lambda_n$, then at least one of the two vectors $\mathbf{u}_1^+$ or $\mathbf{u}_1^-$ are violating;
- the same is true if $\lambda_1 = -\lambda_n$, and if there is no eigenvector of λ_n in $\mathbb{R}^n_+$ (e.g. if λ_n is simple and $\mathbf{u}_n$ has entries with different signs).
- Any $\mathbf{v} \in P_- = \left\{\mathbf{x} \in \Delta : \mathbf{u}_i^\top \mathbf{x} = 0 \text{ for all } i \in [k+1\!:\!n]\right\}$ is a violating vector; note that the polytope P_- may be empty.

Even cheaper to obtain are the following positive/negative certificates, which can be used for preprocessing, too: fix an index i and denote by $\mathbf{e}_i$ the i-th column of the identity matrix I_n. Then we have [20, Lemma 4.4]:

- If $Q_{ii} < 0$, then $\mathbf{v} = \mathbf{e}_i$ is a violating vector;

- if $Q_{ii} = 0 > Q_{ij}$, then $\mathbf{v} = (Q_{jj} + 1)\mathbf{e}_i - Q_{ij}\mathbf{e}_j$ is violating;
- if $Q_{ij} \geq 0$ for all j, then $Q \in \mathcal{C}^*$ if and only if $R = [Q_{jk}]_{j,k\neq i}$ is copositive; if $\mathbf{u} = [u_j]_{j\neq i}$ is violating for R, then $\mathbf{v} = \begin{bmatrix} 0 \\ \mathbf{u} \end{bmatrix} \in \mathbb{R}^n_+$ is violating for Q.
- if $Q_{ij} \leq 0 < Q_{ii}$ for all $j \neq i$, then Q is copositive if and only if $T = [Q_{ii}Q_{jk} - Q_{ij}Q_{ik}]_{j,k\neq i}$ is copositive; if $\mathbf{w} = [w_j]_{j\neq i}$ is violating for T, then $\mathbf{v} = \begin{bmatrix} -\sum_{j\neq i} Q_{ij}w_j \\ Q_{ii}\mathbf{w} \end{bmatrix} \in \mathbb{R}^n_+$ is violating for Q.
- if $Q_{ij} < -\sqrt{Q_{ii}Q_{jj}} < 0$, then $\mathbf{v} = \sqrt{Q_{jj}}\,\mathbf{e}_i + \sqrt{S_{ii}}\,\mathbf{e}_j$ is violating.

After these tests and dropping appropriate rows/columns, it remains to test copositivity of a (possibly smaller) matrix S where *(i)* all diagonal entries are strictly positive; *(ii)* the sign of off-diagonal entries changes in every row; and *(iii)* every (negative) entry $S_{ij} \geq -\sqrt{S_{ii}S_{jj}}$.

6. Applications of copositive optimization

This section will address some typical applications. Before doing that, let us briefly mention other topics (and group related references) which cannot be extensively covered here; for a more extensive, clustered list of references we again refer to [26].

The by now classical role of copositivity for issues of (linear) complementarity and feasibility, some involving also (Markovian) decision problems, is investigated, e.g. in [61, 62, 70, 95, 101]. An interesting application to Simpson's paradox can be found in [69], while the connection of copositivity with conic geometry and angles is discussed, mostly from an optimization perspective, in [5, 65, 78, 110].

The central solution concepts in (evolutionary) game theory, evolutionarily and/or neutrally stable strategies, are both refinements of the Nash equilibrium concept. They are closely connected to copositivity, as shown, e.g., in [10, 14]. But copositivity plays also an important role for modelling friction and contact problems in rigid body mechanics [2, 3, 82, 85]; and, last but not least, for network (stability) problems in queueing, traffic, and reliability [75, 83, 88, 98, 99].

6.1. Convex underestimation in QPs: role of copositivity

In a very recent paper [90], best convex quadratic underestimators g_P of nonconvex functions $f(\mathbf{x}) = \mathbf{x}^\top Q\mathbf{x}$ over polytopes $P = \text{conv}\ \{\mathbf{v}_1, \dots, \mathbf{v}_n\} \subset \mathbb{R}^d$ are studied. So $g_P(\mathbf{x}) = \mathbf{x}^\top S\mathbf{x} + 2\mathbf{c}^\top\mathbf{x} + \gamma$ with $S \in \mathcal{P}$ shall satisfy the underestimation condition $f(\mathbf{x}) \geq g_P(\mathbf{x})$ for all $\mathbf{x} \in P$. To obtain the tightest underestimator of this type, we minimize the *convexity gap*, which is a cumulative measure for deviation of g_P from f based on the volume between the function graphs.

To be more precise, collect again $V = [\mathbf{v}_1, \dots, \mathbf{v}_n]$ in a $d \times n$ matrix and use the Bézier/Bernstein representation of f over P:

$$f(\mathbf{x}) = q_P(\mathbf{v}) = \mathbf{v}^\top Q_P \mathbf{v} \quad \text{with} \quad Q_P = V^\top Q V \quad \text{and} \quad \mathbf{v} \in \Delta \subset \mathbb{R}^n\,.$$

Then search for g_P (or r_P) with

$$f(\mathbf{x}) = q_P(\mathbf{v}) \geq r_P(\mathbf{v}) = \mathbf{v}^\top U_P \mathbf{v} = g_P(\mathbf{x}) \quad \text{for all } \mathbf{x} \in P\,.$$

Again, r_P is the Bézier/Bernstein representation of g_P over P so that

$$U_P = U_P(S, \mathbf{c}, \gamma) = V^\top S V + (V^\top \mathbf{c})\mathbf{e}^\top + \mathbf{e}(V^\top \mathbf{c}) + \gamma E$$

(recall $\mathbf{e} = [1, \dots, 1]^\top \in \mathbb{R}^n$ and $E = \mathbf{e}\mathbf{e}^\top$). Note that U_P is linear in $(S, \mathbf{c}, \gamma)$.

So $f(\mathbf{x}) \geq g_P(\mathbf{x})$ for all $\mathbf{x} \in P$ means $q_P(\mathbf{v}) \geq r_P(\mathbf{v})$ for all $\mathbf{v} \in \Delta$, and by positive homogeneity, this is equivalent to

$$\mathbf{v}^\top (Q_P - U_P)\mathbf{v} = q_P(\mathbf{v}) - r_P(\mathbf{v}) \geq 0 \quad \text{for all } \mathbf{v} \in \mathbb{R}^n_+\,,$$

i.e., $X = Q_P - U_P \in \mathcal{C}^*$. Then the above addressed convexity gap is given by the volume difference

$$\int_\Delta \mathbf{v}^\top (Q_P - U_P)\mathbf{v}\, \mathrm{d}\mathbf{v} = \int_\Delta [q_P(\mathbf{v}) - r_P(\mathbf{v})]\, \mathrm{d}\mathbf{v}\,,$$

and we search for $(S, \mathbf{c}, \gamma) \in \mathcal{P} \times \mathbb{R}^{d+1}$ such that this integral is minimized. Using $\int_\Delta \mathbf{v}^\top X \mathbf{v}\, \mathrm{d}\mathbf{v} = \frac{1}{(n+1)!} \langle E + I, X\rangle$ for any X (this is a small correction of the formula in [90]), we arrive at the problem

$$\begin{array}{lll} \text{minimize} & \langle E + I, X\rangle & \text{(convexity gap)} \\ \text{such that} & X = Q_P - U_P(S, \mathbf{c}, \gamma)\,, & \text{(barycentric coordinates)} \\ & (S, \mathbf{c}, \gamma) \in \mathcal{P} \times \mathbb{R}^d \times \mathbb{R}\,, & \text{(convexity)} \\ & X \in \mathcal{C}^*\,, & \text{(underestimation)}\,, \end{array}$$

which lends itself naturally to the zero-order relaxation of $\mathcal{C}^*$ like $X \in \mathcal{P} + \mathcal{N}$. Higher-order approximations as in Section 3.1 also lead to (larger) SDPs which may yield tighter bounds. For further applications of copositivity to majorization and/or bounding we refer to [29, 103].

6.2. Finding Lyapunov functions for switched systems via copositivity

This is an application of copositivity in the domain of dynamical systems and optimal control. Consider a linear system of ordinary differential equations in the form

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) \quad \text{with } \mathbf{x}(0) = \mathbf{x}_0 \,.$$

This system is asymptotically stable if there is a quadratic Lyapunov function $\mathbf{x}^\top P\mathbf{x}$ where P is positive-definite. This is the case if and only if $AP + PA$ is negative-definite. However, in optimal control we often have additional constraints on the trajectories like $C\mathbf{x}(t) \geq \mathbf{o}$. For this type of dynamical system, the above definiteness criterion on P is too strict. More generally let us follow the lines of [32], and pass to switched systems

$$\dot{\mathbf{x}}(t) = A_i\mathbf{x}(t) \quad \text{such that } C_i\mathbf{x}(t) \geq \mathbf{o}\,, \qquad \text{with } \mathbf{x}(0) = \mathbf{x}_0\,, i = 1, 2\,.$$

We have to find a matrix P such that $\mathbf{x}^\top P\mathbf{x} > 0$ and $\mathbf{x}^\top(A_iP + PA_i)\mathbf{x} < 0$ for all $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{o}\}$ with $C_i\mathbf{x} \geq \mathbf{o}$. Now [32] suggests to proceed similarly as in Section 5.2: suppose that the collections $\mathcal{D}_i$ form a simplicial decomposition of the compact basis B_i for the feasible cones based upon the ℓ^1-sphere:

$$B_i = \{\mathbf{x} \in \mathbb{R}^n : C_i\mathbf{x} \geq \mathbf{o}\,, \|\mathbf{x}\|_1 = 1\}\ ,$$

and collect in V_i the set of all vertices of simplices in $\mathcal{D}_i$, as well as in E_i the set of all (undirected) edges of simplices in $\mathcal{D}_i$. Then P satisfies the above stability condition if and only if P solves the following system of strict linear inequalities for some suitable simplicial decompositions $\mathcal{D}_i$:

$$\left.\begin{array}{rcll} \mathbf{v}^\top P\mathbf{v} & > & 0 & \text{for all } \mathbf{v} \in V_1 \cup V_2 \\ \mathbf{u}^\top P\mathbf{v} & > & 0 & \text{for all } \{\mathbf{u}, \mathbf{v}\} \in E_1 \cup E_2 \\ \mathbf{v}^\top(A_iP + PA_i)\mathbf{v} & < & 0 & \text{for all } \mathbf{v} \in V_i\,,\ i = 1, 2\,, \\ \mathbf{u}^\top(A_iP + PA_i)\mathbf{v} & < & 0 & \text{for all } \{\mathbf{u}, \mathbf{v}\} \in E_i\,,\ i = 1, 2\,. \end{array}\right\}$$

Any solution P to the above system provides a constructive approach to establishing asymptotic stability. In [32] also a negative criterion is formulated. This reduction to a finite system resolves the existence question of copositive quadratic Lyapunov functions, posed as an open problem in [38]. Other applications of copositivity in the domain of dynamical systems and optimal control are covered, e.g., in [28, 42, 79, 84, 97, 115, 125].

6.3. Combinatorial problems from a copositive perspective

The Maximum (Weight) Clique Problem amounts to finding a largest (or heaviest) clique in an undirected graph G (with weights on the n vertices). This NP-complete problem was historically the first for which a copositive representation was suggested [19]. Using an StQP (4) formulation going back to [100] and applying some regularization [12], one arrives at the copositive formulation

$$\tfrac{1}{\omega(G)} = \alpha_{Q_G} = \min \left\{ \langle Q_G, X \rangle : \langle E, X \rangle = 1 \, , \; X \in \mathcal{C} \right\} \, , \tag{30}$$

where Q_G is a matrix derived from the adjacency matrix of G (and the weights). Taking the inverse $t = \frac{1}{y}$ in the dual of the rightmost problem above, we also arrive at the formulation of [48] (for the complementary graph):

$$\omega(G) = \min \left\{ t : tQ_G - E \in \mathcal{C}^* \right\} \, .$$

Here $\omega(G)$ is the clique number of G, i.e., the size (weight) of a maximum (weight) clique in G. Replacing $\mathcal{C}^*$ with its zero-order approximation, we get a strengthening $\theta'(G)$ of the well-known Lovász bound $\theta(G)$ [91, 96, 119]:

$$\theta'(G) = \min \left\{ t : tQ_G - E \in \mathcal{P} + \mathcal{N} \right\} \geq \omega(G) \, ,$$

while shrinking further the feasible set to $\mathcal{P}$, we finally arrive at the Lovász number $\theta(G)$ which – like $\theta'(G)$ – can be computed in polynomial time:

$$\theta(G) = \min \left\{ t : tQ_G - E \in \mathcal{P} \right\} \geq \theta'(G) \geq \omega(G) \, .$$

Strong duality yields, as above,

$$\tfrac{1}{\theta'(G)} = \min \left\{ \langle Q_G, X \rangle : \langle E, X \rangle = 1 \, , \; X \in \mathcal{P} \cap \mathcal{N} \right\} \, ,$$

and a recent improvement over $\theta'(G)$ adding a single valid cut motivated by the copositive representation is

$$\tfrac{1}{\theta^C(G)} = \min \left\{ \langle Q_G, X \rangle : \langle E, X \rangle = 1 \, , \; \langle C, X \rangle \geq 0 \, , \; X \in \mathcal{P} \cap \mathcal{N} \right\} \geq 1/\theta'(G) \, ,$$

where $C \in \mathcal{C}^*$ is arbitrary: indeed, for any $X \in \mathcal{C}$ we then have $\langle C, X \rangle \geq 0$. See [21] for appropriate choices of C and results. Similar ideas are followed in [4, 36, 35, 54, 55], while an approach by warm-starting methods is presented in [60].

Higher-order approximation alternatives, with a particular emphasis on SDP-based bounds on the clique number can be found in [48, 109, 86]. Similar copositive optimization approaches, among many others, were employed to obtain bounds on the (fractional) chromatic number of a graph [56]. Further applications of copositive optimization to graph theory and other discrete problems can be found, e.g., in [87, 121].

In [67] the following copositive formulation of the chromatic number $\chi(G)$ of a graph is proposed:

$$\chi(G) = \max_{(y,z)\in\mathbb{R}^2} \left\{ y : \tfrac{t-y}{n^2} E + zn(I + A_{G_t})E \in \mathcal{C}^* \text{ for all } t \in [1\!:\!n] \right\} ,$$

where A_{G_t} is the adjacency matrix of the cartesian product $G_t = K_t \otimes G$, with K_t denoting the complete graph on t vertices. Other combinatorial problems also have a copositive formulation of a similar (although somehow smaller) product type: the problem of graph partitioning [111] and the quadratic assignment problem (QAP) [112]. The latter is encoded as follows as a copositive optimization problem: for a QAP instance (A, B, C) and a symmetric $n^2 \times n^2$ matrix Y with $(i, j)-$th block Y^{ij} of order $n\times n$, denote by $\mathbf{c} = \text{vec}\, C \in \mathbb{R}^{n^2}$. Then the QAP can be written as

$$\begin{array}{ll} \text{minimize} & \langle B \otimes A + \text{Diag}\, \mathbf{c}, Y\rangle \\ \text{such that} & \sum_i Y^{ii} = I_n \,, \\ & \langle I_n, Y^{ij}\rangle = \delta_{ij} \quad \text{for all } \{i, j\} \subseteq [1\!:\!n] \,, \\ & \langle E, Y\rangle = n^2 \,, \\ & Y \in \mathcal{C} \,. \end{array}$$

6.4. A success story: improving bounds on crossing numbers by copositivity

A particularly hard combinatorial problem is to determine the crossing number $\text{cr}(G)$ of a graph G, i.e. to find the minimal number $\text{cr}(G)$ of edge crossings in a planar drawing of G (note that this planar drawing does not result automatically if $\text{cr}(G)$ is known). Even for such small graphs G as K_{13} or $K_{7,11}$, the crossing number is still unknown. As usual $K_{n,m}$ denotes the complete bipartite graph with class sizes n and m. Arranging the first class horizontally and the second vertically in a symmetric manner, it is easy to see that $\text{cr}(K_{n,m}) \geq Z(m, n)$ where

$$Z(m, n) = \left\lfloor (m-1)^2/4 \right\rfloor \left\lfloor (n-1)^2/4 \right\rfloor$$

is the number which Kazimierz Zarankiewicz conjectured in [127] to give the crossing number $\text{cr}(K_{n,m})$. In 1977, Pál Turán remembered [122] that he and Zarankiewicz worked on this problem in a concentration camp near Budapest, under forced labor, to minimize crossings of a railway system in brick production (every crossing involved danger of derailing, which was cruelly punished). Now [47] constructed a $k \times k$ matrix Q_m (transposition distances of cyclic permutations) with $k = (m-1)!$ such that the crossing number can be estimated by the optimal value $\alpha_{Q_m} = \min\left\{\mathbf{x}^\top Q_m \mathbf{x} : \mathbf{x} \in \Delta\right\}$ of the StQP based upon Q_m:

$$\operatorname{cr}(K_{m,n}) \geq \frac{n}{2}\left(n\,\alpha_{Q_m} - \lfloor (m-1)^2/4 \rfloor\right) .$$

For $m = 9$ we have $k = 40320$, and [50] used advanced copositive optimization techniques, exploiting symmetries and SDP technology, to obtain a lower bound for α_{Q_m}, to arrive for even n at the estimate

$$4\,n^2 - 8n \geq \operatorname{cr}(K_{9,n}) \geq \frac{n}{2}\left(n\alpha_{Q_9} - 16\right) \geq 3.8676\,n^2 - 8n$$

and for odd n at the estimate

$$4\,n^2 - 8n + 15 \geq \operatorname{cr}(K_{9,n}) \geq \frac{n}{2}\left(n\alpha_{Q_9} - 16\right) \geq 3.8676\,n^2 - 8n\,.$$

Using the relation $\operatorname{cr}(K_{m,n}) \geq \frac{m(m-1)}{r(r-1)} \operatorname{cr}(K_{r,n})$ for all $r \leq m$, and putting $r = 9$, these estimates have the asymptotic implication

$$\lim_{n\to\infty} \frac{\operatorname{cr}(K_{m,n})}{Z(m,n)} \geq 0.8594\,\frac{m}{m-1} \quad \text{for all } m \geq 9\,.$$

The best previously known constants were 0.8001 [104] and 0.83 [47]. We also obtain with $Z(n) = \frac{1}{4}\left\lfloor\frac{n}{2}\right\rfloor\left\lfloor\frac{n-1}{2}\right\rfloor\left\lfloor\frac{n-2}{2}\right\rfloor\left\lfloor\frac{n-3}{2}\right\rfloor$

$$\lim_{n\to\infty} \frac{\operatorname{cr}(K_n)}{Z(n)} \geq \lim_{n\to\infty} \frac{\operatorname{cr}(K_{n,n})}{Z(n,n)} \geq 0.8594\,,$$

and again the constant on the right-hand side is the best known up to now. For very recent, significant improvements in runtime via symmetry arguments to obtain these bounds we refer to [46, 52].

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