OPTIMA 89

Mathematical Optimization Society Newsletter

Philippe L. Toint

MOS Chair's Column

August 1, 2012. While preparing this column and in my periodic and frantic search for material of interest, I stumbled on this most appropriate motto: *Optimum is maximum at a minimum* – due to the nu-jazz artist Mr Gaus (no, this is not made up). In view of the coming ISMP festivities, this sounded a marvelous quote, at least if properly interpreted. Indeed, it would be completely wrong to suggest that "Optimum is maximum at a minimum in Berlin", with the implication that the next ISMP is a minimum! In fact it is truly the opposite: a global maximum in the history of major MOS meetings. The latest numbers sent to me by Martin Skutella, the very active chair of the organization committee, show that the next ISMP will feature more than 1700 talks and about 600 invited and contributed sessions in 24 program clusters! The downside of this resounding success is that 40 parallel tracks will be necessary ... You will also be approximately 2000 participants from more than 60 countries from all over the world. ISMP 2012 will thus be the biggest ISMP so far, and I am of course looking forward to meeting so many of you there very soon.

The end of the "inter-ISMP" period is also bringing some changes in the organization of the Society, with the renewal of the Council and the election of a new chair-elect and treasurer. It is my very great pleasure to announce that the new chair elect is Bill Cook, who will serve as MOS Vice-Chair up to August 31st, 2013, after that he will be taking over from me as MOS Chair for three years. Juan Meza, our present efficient treasurer, has been reconducted for a second term. On the Council side, new Council members will start their term after the ISMP 2012. These are Miguel Anjos, Sam Burer, Volker Kaibel and Alejandro Joffre. I wish to congratulate them all for their election and I am truly looking forward to work with them in the coming year.

This is also the occasion of many thanks. First, I wish to express my deep gratitude to Steve Wright, whose term as Vice-Chair is ending this summer, after many years at the service of our Society. Steve's help and advice have been invaluable in the conduct of MPS and then MOS. His experience, memory and judgement have helped me, the Executive Committee and the Council very significantly. Many many thanks, dear Steve.

Real thanks are also due to Kurt Anstreicher, who will pass on the job of Editor in Chief of *Mathematical Programming A* to Alexander Shapiro on September 1st, 2012. Kurt has been very instrumental in keeping our flagship journal at the top of our scientific field, a "strong hand in a velvet glove". His action at MPA has been unanimously appreciated. I am glad to say that Kurt will continue to serve the Society as Chair of the Executive Committee, where he is already of very great help. Thank you, Kurt. And also thank you Alex for accepting the responsibility of being the new MPA EIC.

Due to these various nominations, some change has also become necessary in the MOS Publications Committee. Alex Shapiro is stepping down as chairman and member of this committee (again many thanks, Alex) and Nick Gould will take this position on from September 1st, with the help of Christoph Helmberg, Jie Sun, Robert Weismantel and Darinka Dentcheva, who has just accepted to join. Thank you in advance to Nick and Darinka for their new commitment.

My final thanks go to the Council members whose term is ending: Jeff Linderoth, Claudia Sagastizabal, Martin Skutella and Luis Vicente. Their continued advice and input have been of great help over the past three years.

Unfortunately, this column also contains very sad news. We learned with stupor that Alberto Caprara, one of our distinguished and brilliant colleagues, died in April in a hiking accident in the Dolimiti. Alberto served the Society as an Optima co-editor and will be deeply missed by many of us.

To conclude on a positive mood, the MOS members may have noticed that the Society is reaching its 40 years! Indeed, according to the history notes available on the MOS website, 366 Charter Members were enrolled in early 1972, who then adopted a Constitution of what became the *Mathematical Programming Society* and later the *Mathematical Optimization Society*. So, happy birthday MOS and you all!

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Note from the Editors

We introduce our latest issue of Optima dedicated to the topic of copositive programming, an interesting and fast-growing topic in optimization. The main article is an extensive survey by Immanuel M. Bomze, Mirjam Dür, and Chung-Piaw Teo. The accompanying discussion column is by Monique Laurent.

This issue is scheduled to be published on the eve of ISMP 2012 in Berlin and will be followed by *Optima@ISMP* – an exciting and entertaining daily publication established at the last ISMP 2009 in Chicago.

We cannot conclude without mentioning the extremely sad event of Alberto Caprara's passing last April, which is by now known by many colleagues and is particularly noted by the Optima team since Alberto was a past Optima editor. While his obituary will be published in one of the issues of *Optima@ISMP* we wanted to announce our plans to publish in the near future an issue of this regular Optima newsletter dedicated to Alberto's extensive contributions.

Sam Burer,
Volker Kaibel
and Katya Scheinberg
Optima editors

Immanuel M. Bomze, Mirjam Dür, and Chung-Piaw Teo

Copositive Optimization

1 Introduction

Copositive optimization means minimizing a linear function in matrix variables subject to linear constraints and the constraint that the matrix should be in the convex cone $\mathcal{C}^n$ of *copositive matrices*

$$\mathcal{C}^n = \{S \in \mathcal{S}^n : x^\top S x \geq 0 \text{ for all } x \in \mathbb{R}^n_+\}.$$

Here $\mathcal{S}^n$ denotes the set of symmetric matrices, and $\mathbb{R}^n_+$ the nonnegative orthant. Associated to such a problem is a dual problem which involves the constraint that the dual variable lies in the dual cone of $\mathcal{C}^n$, that is, the convex cone $\mathcal{C}^{n*}$ of *completely positive matrices*:

$$\mathcal{C}^{n*} = \operatorname{conv}\{xx^\top : x \in \mathbb{R}^n_+\}.$$

The concept of copositivity goes back to Motzkin [39] in 1952. Since then, both copositivity and complete positivity have been investigated in great detail by matrix theorists, see [1] or [27] for surveys. The use of the two cones in optimization has been discovered only recently, starting with a paper by Quist et al. [44] from 1998 who suggested that semidefinite relaxations of quadratic problems may be tightened by looking at the (dual of the) copositive cone.

Bomze et al. [5] were the first to establish an equivalent copositive formulation of an NP-hard problem, namely the standard quadratic problem. Their paper from 2000 also coined the term "copositive programming". Since then, a number of other quadratic and combinatorial problems have also been studied from the copositive viewpoint which has opened a completely new way to deal with these problems. In 2009, Burer gave a fundamental representation result [12] which states that any problem with a quadratic objective, linear constraints and possibly binary variables can equivalently be formulated as a copositive optimization problem. This representation result gave a real boost to the field and has opened a whole new approach to many quadratic and combinatorial problems, yielding both a better theoretical understanding and often stronger bounds on the problems.

In this paper, we highlight some recent developments in this young but highly active and promising field. We discuss how to model a quadratic or combinatorial problem as well as problems involving data uncertainty as copositive problems; we list known properties of the copositive cone as well as several open questions; and we discuss algorithmic approaches and a variety of approximation hierachies.

We also mention that several more detailed surveys on copositive optimization have appeared recently, see [3, 13, 23].

2 Modelling problems as copositive or completely positive problems

In this section, we discuss how copositivity can be used to model various NP-hard optimization problems. We begin with deterministic problems.

2.1 Deterministic quadratic and combinatorial problems

We start by illustrating the connection between copositive and quadratic optimization by means of the so called standard quadratic problem (with $e = [1, \dots, 1]^\top \in \mathbb{R}^n$)

$$(\text{StQP}) \qquad \begin{array}{ll} \min & x^\top Q x \\ \text{s.t.} & e^\top x = 1, \\ & x \in \mathbb{R}^n_+. \end{array}$$

This optimization problem asks for the minimum of a (not necessarily convex) quadratic function over the standard simplex $\Delta^n = \{x \in \mathbb{R}^n_+ : e^\top x = 1\}$. It is known that this problem is NP-hard, since it contains the maximum clique as a special case: consider a graph G with adjacency matrix A_G and denote its clique number by $\omega(G)$. It was shown by Motzkin and Straus [35] that then

$$\frac{1}{\omega(G)} = \min\{x^\top(E - A_G)x : x \in \Delta^n\},$$

where $E = ee^\top$ is the $n \times n$ matrix of all ones.

Easy manipulations show that the objective function of (StQP) can be written as $x^\top Q x = \langle Q, xx^\top \rangle$ where $\langle X, Y \rangle = \operatorname{trace}(XY)$ for $\{X, Y\} \subset \mathcal{S}^n$. Analogously the constraint $e^\top x = 1$ transforms to $\langle E, xx^\top \rangle = 1$. Hence, the problem

$$\begin{array}{ll} \min & \langle Q, X \rangle \\ \text{s.t.} & \langle E, X \rangle = 1, \\ & X \in \mathcal{C}^{n*} \end{array} \tag{1}$$

is obviously a relaxation of (StQP). Since the objective is now linear, an optimal solution must be attained in an extremal point of the convex feasible set. It is not difficult to show that these extremal points are precisely the rank-one matrices $xx^\top$ with $x \in \Delta^n$. Together, these results imply that (1) is in fact an exact reformulation of (StQP), as was shown in [5].

The remarkable point in this representation is that we have transformed the NP-hard standard quadratic problem into a linear problem with an additional convex constraint (recall that $\mathcal{C}^{n*}$ is a convex set!). And in contrast to the countless SDP relaxations out there, this copositive formulation is not a relaxation but an exact reformulation in the sense that (StQP) and (1) have the same optimal values, and any optimal solution $\bar{X}$ of (1) is in the convex hull of the matrices $\bar{x}\bar{x}^\top$, where $\bar{x}$ is an optimal solution of (StQP). This immediately shows that the complexity must now be hidden in the cone constraint, and indeed checking membership in both $\mathcal{C}^n$ and $\mathcal{C}^{n*}$ is NP-hard, see [18, 36].

Burer [12] extended the above and gave a celebrated representation result which states that every quadratic problem of the form

$$\begin{array}{lll} \min & x^\top Q x + 2c^\top x & \\ \text{s.t.} & a_i^\top x = b_i \quad (i = 1, \dots, m) & \\ & x \in \mathbb{R}^n_+ & \\ & x_j \in \{0, 1\} \quad (j \in B \subseteq \{1, \dots, n\}) & \end{array} \tag{2}$$

can equivalently be reformulated as the following completely positive problem:

$$\begin{aligned} \min \quad & \langle Q, X\rangle + 2c^\top x \\ \text{s.t.} \quad & a_i^\top x = b_i \quad (i = 1,\dots,m) \\ & \langle a_i a_i^\top, X\rangle = b_i^2 \quad (i = 1,\dots,m) \\ & x_j = X_{jj} \quad (j \in B) \\ & \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \in \mathcal{C}^{n+1*}, \end{aligned}$$

provided that (2) satisfies the so-called key condition, i.e.,

$$a_i^\top x = b_i \text{ for all } i \text{ and } x \in \mathbb{R}_+^n \text{ implies } x_j \le 1 \text{ for all } j \in B\,.$$

This condition can always be enforced by introducing slack variables if necessary. A weaker version of this condition is studied by Bomze and Jarre in [6].

Copositive formulations have been proposed and used also for many combinatorial problems. For these, we refer to the surveys [3, 23] and references there; see also the clustered bibliography on copositivity in [8].

2.2 *Modelling uncertainty*

Burer's result can be extended to stochastic mixed-binary linear optimization problems with objective uncertainty. We review the results and some recent applications in this section.

Consider a mixed-binary linear problem in maximization form:

$$Z(c) = \max\{c^\top x \;:\; x \in F\} \tag{3}$$

where the feasible region F is described as:

$$F = \Big\{x \in \mathbb{R}_+^n : \;\; a_j^\top x = b_j, \text{ for } j = 1,\dots,m, \;\; x_i \in \{0,1\}, \text{ for } i \in B\Big\} \tag{4}$$

with $B \subseteq \{1,\dots,n\}$ designating a fixed subset indexing the binary variables. We assume further that the constraints in F are such that the only solution in F when $b_j = 0$ for all j is $x_i = 0$ for all i.

Consider the following problem that arises in probabilistic analysis of mixed binary linear problems:

Given the mixed binary linear problem (3) and a probability measure θ for the random objective coefficient vector $\tilde{c}$, compute the expected optimal value:

$$\text{(Mean)} \qquad \mathbb{E}_\theta\left[Z(\tilde{c})\right] = \int Z(c)\,\mathrm{d}\theta(c)\,.$$

Clearly, computing (Mean) is at least as hard as solving the deterministic optimization problem. It is computable in time polynomial in the size of the problem if the deterministic problem is solvable in polynomial time and θ is a discrete distribution with a polynomial number of support points. However, in the general case, the exact computation of (Mean) can be significantly more challenging than solving the deterministic problem. Lovász [32] showed that a bound for this problem can be obtained via solving a related convex program, using the fact that the marginal distributions are log-concave, for certain classes of polyhedra. However, Natarajan, Teo and Zheng [38] were able to extend Burer's result to mixed-binary linear problems with objective uncertainty, and obtained a more general bound, using a copositive formulation. This bound is weaker than Lovász' for the class of log-concave marginal distributions on certain polyhedra, since it uses only the first and second moments information.

Theorem 1. *Let Θ be the set of distributions for a nonnegative random vector $\tilde{c}$ with prescribed first moment vector μ, and second moment matrix Π. Then $\sup\limits_{\theta\in\Theta} \mathbb{E}_\theta\left[\max\limits_{x\in F} \tilde{c}^\top x\right]$ can be obtained by solving*

$$\begin{aligned} \max \quad & \sum_{i=1}^n Y_{ii} \\ \text{s.t.} \quad & a_j^T x = b_j && \text{for } j = 1,\dots,m \\ & a_j^T X a_j = b_j^2 && \text{for } j = 1,\dots,m \\ & X_{ii} = x_i && \text{for } i \in B \subseteq \{1,\dots,n\} \\ & \begin{bmatrix} 1 & \mu^\top & x^\top \\ \mu & \Pi & Y^\top \\ x & Y & X \end{bmatrix} \in \mathcal{C}^{2n+1*}. \end{aligned} \tag{5}$$

The decision variables in this formulation are defined as:

$$\begin{aligned} x &= \mathbb{E}\left[x(\tilde{c})\right] \\ Y &= \mathbb{E}\left[x(\tilde{c})\tilde{c}^\top\right] \\ X &= \mathbb{E}\left[x(\tilde{c})x(\tilde{c})^\top\right]. \end{aligned}$$

The objective function is expressed as:

$$\mathbb{E}\left[Z(\tilde{c})\right] = \sum_{i=1}^n \mathbb{E}\left[\tilde{c}_i x_i(\tilde{c})\right] = \sum_{i=1}^n Y_{ii}$$

The first two constraints in formulation (5) are from taking the expectation of the equality constraints:

$$\begin{aligned} \mathbb{E}\left[a_j^\top x(\tilde{c})\right] &= a_j^\top x &&= b_j \\ \mathbb{E}\left[\left(a_j^\top x(\tilde{c})\right)^2\right] &= a_j^\top X a_j &&= b_j^2\,. \end{aligned}$$

The third constraint is from taking the expectation of the equality constraint $x_i(\tilde{c})^2 = x_i(\tilde{c})$ for the binary variables:

$$X_{ii} = \mathbb{E}\left[x_i(\tilde{c})^2\right] = \mathbb{E}\left[x_i(\tilde{c})\right] = x_i\,.$$

The validity of the cone constraint follows from $\{x(\tilde{c}), \tilde{c}\} \subseteq \mathbb{R}_+^n$ and from the moment representation

$$\begin{aligned} \begin{bmatrix} 1 & \mu^\top & x^\top \\ \mu & \Pi & Y^\top \\ x & Y & X \end{bmatrix} &= \begin{bmatrix} 1 & [\mathbb{E}(\tilde{c})]^\top & \mathbb{E}\left[x(\tilde{c})\right]^\top \\ \mathbb{E}(\tilde{c}) & \mathbb{E}\left(\tilde{c}\tilde{c}^\top\right) & \mathbb{E}\left[\tilde{c}x(\tilde{c})^\top\right] \\ \mathbb{E}\left[x(\tilde{c})\right] & \mathbb{E}\left[x(\tilde{c})\tilde{c}^\top\right] & \mathbb{E}\left[x(\tilde{c})x(\tilde{c})^\top\right] \end{bmatrix} \\ &= \mathbb{E}\begin{bmatrix} 1 & \tilde{c}^\top & x(\tilde{c})^\top \\ \tilde{c} & \tilde{c}\tilde{c}^\top & \tilde{c}x(\tilde{c})^\top \\ x(\tilde{c}) & x(\tilde{c})\tilde{c}^\top & x(\tilde{c})x(\tilde{c})^\top \end{bmatrix} \in \mathcal{C}^{2n+1*}. \end{aligned}$$

As a (limit of) convex combination(s) of completely positive matrices, this matrix is itself completely positive. While the number of constraints and variables are polynomial size, the difficulty lies in the cone constraint. The proof of tightness can be found in [38]. Note that the model constructed this way also gives us the estimates of $\mathbb{E}\left[x_i(\tilde{c})\right]$ for the worst case distribution. This provides an estimate to $\mathbb{P}(x_i(\tilde{c}) = 1)$ in $Z(\tilde{c})$, when $i \in B$. This is the persistency problem studied in [2] and [37], using only the marginal moments and distributional information.

As an immediate application, consider the case when

$$F = \{x \in \Delta^n : x_i \in \{0,1\} \text{ for all } i \in \{1,\dots,n\}\}\,,$$

where $\sup\limits_{\theta\in\Theta} \mathbb{E}_\theta\left[\max\limits_{x\in F} \tilde{c}^\top x\right]$ reduces to a classical order statistics problem of finding $\sup\limits_{\theta\in\Theta} \mathbb{E}_\theta\left[\max\{\tilde{c}_1,\dots,\tilde{c}_n\}\right]$. For this class of problems, the matrix X in (5) can be assumed to be diagonal. Interestingly, for this problem, using a result in [20], it follows that

$$\begin{bmatrix} 1 & \mu^\top & x^\top \\ \mu & \Pi & Y^\top \\ x & Y & X \end{bmatrix} \in \mathcal{C}^{d*} \Leftrightarrow \begin{bmatrix} 1 & \mu^\top & x^\top \\ \mu & \Pi & Y^\top \\ x & Y & X \end{bmatrix} \in \mathcal{P}^d \cap \mathcal{N}^d, \tag{6}$$

where $\mathcal{P}^d$ denotes the cone of all positive-semidefinite (psd) symmetric $d \times d$ matrices, and $\mathcal{N}^d$ all symmetric $d \times d$ matrices with no negative entry, and $d = 2n + 1$ here.

The upper bound on the order statistics problem can now be solved as a semidefinite optimization problem (SDP). We give an illustration of this result (see [34], where the problem is cast as an SDP termed CMM): Suppose X_i are i.i.d. random variables with mean μ_i and standard deviation σ_i. Let

$$S_k = X_1 + \ldots + X_k, \quad k = 1, \ldots, n,$$

with $S_0 = 0$. The goal is to estimate the probability that the random walk attains its maximum value at step k, i.e., find

$$\mathbb{P}\left[S_k = \max_{0 \le j \le n} S_j \right].$$

If the X_i's are independent, this probability can be rewritten as:

$$\begin{aligned}
&\mathbb{P}\left[S_k = \max_{0 \le j \le n} S_j \right] \\
&= \mathbb{P}\left[X_k \ge 0, \sum_{j=k-1}^{k} X_j \ge 0, \ldots, \sum_{j=1}^{k} X_j \ge 0 \right] \times \\
&\qquad \times \mathbb{P}\left[X_{k+1} \le 0, \ldots, \sum_{j=k+1}^{n} X_j \le 0 \right] \\
&= \mathbb{P}\left[S_1 \ge 0, S_2 \ge 0, \ldots, S_k \ge 0 \right] \times \mathbb{P}\left[S_1 \le 0, \ldots, S_{n-k} \le 0 \right].
\end{aligned}$$

Let $\alpha = \frac{1}{n} \sum_{i=1}^{n} \mathbb{P}(S_i > 0)$. Then the classical arcsine law states that the probability

$$\mathbb{P}\left[S_k = \max_{0 \le j \le n} S_j \right] \sim \frac{1}{n\pi} \sin(\alpha\pi) \left(\frac{k}{n} \right)^{\alpha - 1} \left(1 - \frac{k}{n} \right)^{-\alpha} \quad \text{for large } n.$$

Contrary to popular intuition, the two end points ($k = 0$ or $k = n$) have the highest probability of attaining the maximum.

The above is identical to an order statistics problem, where the kth measurement is given by the summand $S_k = \sum_{j=1}^{k} X_k$. We can obtain the choice probability estimates using the completely positive cone (and solving an SDP), with $\mu_k = \mathbb{E}(S_k) = \sum_{j \le k} \mu_j$ and

$$\Pi_{ij} = \mathbb{E}(S_i S_j) = \sum_{a \le i, b \le j, a \ne b} \mu_a \mu_b + \sum_{a \le i, j} (\mu_a^2 + \sigma_a^2).$$

The CMM formulation from [34] is able to approximately return the arcsine law behaviour of the choice probabilities, with slight over-estimation for the more probable alternatives ($k = 0$ and $k = n$), and under-estimation for the less probable alternatives ($k \approx n/2$).

The method has also been applied to a more complex class of appointment scheduling problem [28], where F corresponds to a class of minimum cost flow solutions, and the challenge is to schedule the arrival time of a given sequence of patients, each with random consultation time, to minimize the total waiting time of the patients, and the overtime of the doctor. Compared to a state-of-the-art two-stage stochastic optimization method [16], the total waiting time costs under the two schedules obtained by [28] using (single-stage) copositive optimization are quite competitive, in a highly robust way with varying cost structures and waiting time distributions.

3 The cones $\mathcal{C}^n$ and $\mathcal{C}^{n*}$

Now we have seen the potential of copositivity as a modeling tool, let us review some properties of the cones $\mathcal{C}^n$ and $\mathcal{C}^{n*}$.

Both sets are full-dimensional closed, convex, pointed matrix cones. They are non-polyhedral, and their boundaries contain both flat parts and curved parts. See Figure 1 for a picture of $\mathcal{C}^2$.

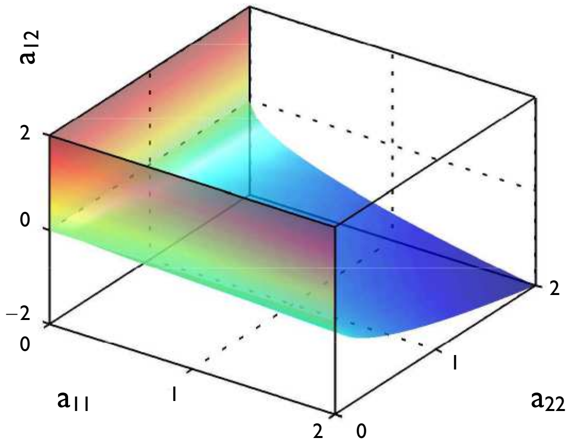


Figure 1. *The cone of copositive 2×2 matrices parametrized by the diagonal elements a_{11} and a_{22} and the off-diagonal element $a_{12} = a_{21}$. Points above the depicted surface represent a copositive matrix.*

We easily see from the definitions that

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

It is a surprising fact (cf. [33]) that for $n \le 4$, we have equality in the relations $\mathcal{C}^{n*} \subseteq \mathcal{P}^n \cap \mathcal{N}^n$ and $\mathcal{P}^n + \mathcal{N}^n \subseteq \mathcal{C}^n$, whereas for $n \ge 5$, both inclusions are strict. A counterexample that illustrates $\mathcal{C}^n \ne \mathcal{P}^n + \mathcal{N}^n$ is the so-called Horn-matrix, cf. [25]:

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix} \in \mathcal{C}^5 \setminus (\mathcal{P}^5 + \mathcal{N}^5). \qquad (7)$$

Figure 2 gives another illustration on the geometry of the cones which has been studied in more detail by Dickinson [17].

3.1 Extremal (generating) rays

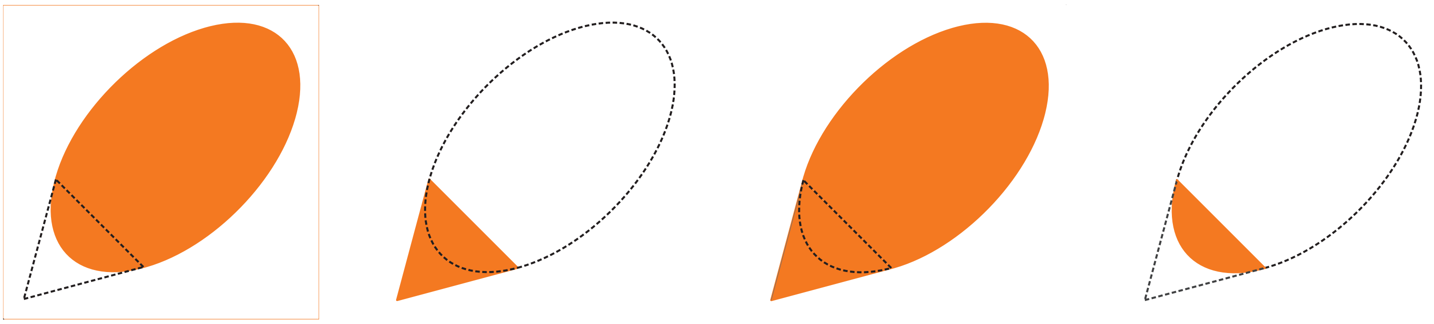
Note that by using the matrix inner product, we can rewrite the definitions of our cones as follows:

$$\begin{aligned}
\mathcal{C}^n &= \{ S \in \mathcal{S}^n : \langle S, xx^\top \rangle \ge 0 \text{ for all } x \in \mathbb{R}^n_+ \}, \\
\mathcal{C}^{n*} &= \operatorname{conv}\{ xx^\top : x \in \mathbb{R}^n_+ \}.
\end{aligned}$$

This means that we have an outer description by means of supporting hyperplanes for $\mathcal{C}^n$, and an inner description of $\mathcal{C}^{n*}$ as the convex hull of some set of matrices. It is well known that by duality the extremal matrices of a cone provide an outer description by hyperplanes of its dual cone. From this, we immediately get that the extremal rays of $\mathcal{C}^{n*}$ are given by the rank one matrices $xx^\top$ with $x \in \mathbb{R}^n_+$.

Giving a full characterization of the extremal rays of $\mathcal{C}^n$ (or equivalently, a complete "outer" description of $\mathcal{C}^{n*}$ in terms of supporting hyperplanes) is an open problem. Only recently has this question been answered for the 5×5 case. Before we state this result, first note that for any permutation matrix P and diagonal matrix D with strictly positive diagonal we have equivalence of the following three statements: (a) X is extremal for $\mathcal{C}^n$; (b) $PXP^\top$ is extremal for $\mathcal{C}^n$; and (c) DXD is extremal for $\mathcal{C}^n$. We refer to all matrices generated this way as the "orbit" of X. Now Hildebrand [26] proved the following:

Theorem 2. *A matrix $X \in \mathcal{C}^5$ generates an extremal ray for $\mathcal{C}^5$ if and only if it is in the orbit of a matrix of one of the following forms:*



Semidefinite cone $\mathcal{P}^2$ Nonnegative cone $\mathcal{N}^2$ Copositive cone $\mathcal{C}^2$ Completely positive cone $\mathcal{C}^{2*}$

Figure 2. *The picture illustrates the geometry of the cones for the case of symmetric 2×2 matrices which have three parameters. Here a cross section of each of the resulting cones in $\mathbb{R}^3$ is shown. This case is easy because of $\mathcal{C}^{2*} = \mathcal{P}^2 \cap \mathcal{N}^2$ and $\mathcal{C}^2 = \mathcal{P}^2 \cup \mathcal{N}^2$. In higher dimensions (even for $n = 3, 4$), the geometry is much more complex.*

- E_{ij} *(the 5×5 matrix having zeros everywhere except for ones in positions ij and ji)*
- $aa^\top$ *for some vector $a \in \mathbb{R}^5$ which contains both positive and negative elements*
- *the Horn matrix from (7)*
- *a matrix of the form*

$$\begin{bmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{bmatrix},$$

where the parameters fulfill $\sum_{i=1}^{5} \psi_i < \pi$ and $\psi_i > 0$.

This characterization gives some insight into the complicated structure of $\mathcal{C}^n$. Observe that understanding better the extremal rays of $\mathcal{C}^n$ would also be useful from an algorithmic point of view, since this knowledge could be used to generate cutting planes: Assume we consider a combinatorial problem in its completely positive formulation and relax this to an SDP. An optimal SDP solution will usually not be in $\mathcal{C}^{n*}$, so adding a cut will tighten the SDP relaxation. Such cutting planes correspond to supporting hyperplanes of $\mathcal{C}^{n*}$, or equivalently, extremal matrices of $\mathcal{C}^n$. First attempts to explore this path have been made in [14, 22, 47]. This structure is also exploited in a recent study of $\mathcal{C}^{5*}$ [7].

4 Approximation hierarchies

Since optimization problems over $\mathcal{C}^{n*}$ and $\mathcal{C}^n$ can not be solved directly, it is natural to study inner and outer approximations. Different approaches to this end have been proposed: discretization methods, sum-of-squares conditions, and moment approaches. Whereas the latter two provide uniform approximations (for a recent survey consult [31]), discretization methods can potentially be tailored to provide a good approximation only in the region of the cone that is relevant for the optimization.

We start by discussing discretization methods.

4.1 Discretization methods

For an arbitrary (possibly finite) subset $T \subseteq \mathbb{R}^n_+$, define

$$\operatorname{Pos}(T) := \{S \in \mathcal{S}^n : y^\top S y \geq 0 \text{ for all } y \in T\}.$$

We start with the simple observation that any copositive matrix S satisfies $S \in \operatorname{Pos}(T)$, so we get an outer approximation of $\mathcal{C}^n$ of the type $\mathcal{C}^n \subset \operatorname{Pos}(T)$. Note that $\operatorname{Pos}(T)$ is a polyhedral cone whenever T is a finite set, and that $T_1 \subset T_2$ implies $\operatorname{Pos}(T_1) \supseteq \operatorname{Pos}(T_2)$ so that increasing T will shrink $\operatorname{Pos}(T)$, hopefully tight enough to approximate $\mathcal{C}^n$ well. Also note that for some infinite sets T, this approximation becomes exact, e.g. for any base T of $\mathbb{R}^n_+$ in the sense that $\mathbb{R}_+ T = \mathbb{R}^n_+$ we have $\operatorname{Pos}(T) = \mathcal{C}^n$. Of course, polyhedrality is then lost.

For example, we could use the standard simplex $T = \Delta^n$ as such a base. Note that also other (infinite and/or discrete) sets T may satisfy $\operatorname{Pos}(T) = \mathcal{C}^n$, e.g., $T = \mathbb{N}^n$ (with $\mathbb{N}$ denoting the non-negative integers; apparently this has been first noticed by the authors of [9]; this remark was contained in a related talk but is not made explicit in [9]). A first outer approximation hierarchy is immediate from this: let

$$\mathbb{N}^n_r = \left\{ \mathbf{m} \in \mathbb{N}^n : \sum_{i=1}^{n} m_i = r \right\}$$

and put $\mathcal{I}^n_d = \operatorname{Pos}(\mathbb{N}^n_{d+2})$ (the shift in d is introduced for consistency with the following developments; note that $S \in \operatorname{Pos}(\mathbb{N}^n_1)$ if and only if $\operatorname{diag} S \in \mathbb{R}^n_+$ while $\operatorname{Pos}(\mathbb{N}^n_0) = \mathcal{S}^n$ is truly trivial). The same hierarchy was introduced in [4] via the regular rational grid $\Delta^n_d = \frac{1}{d+2}\mathbb{N}^n_{d+2} \subset \Delta^n$, which has $\binom{n+d+1}{d+2}$ elements:

$$\mathcal{I}^n_d = \operatorname{Pos}(\Delta^n_d), \quad d \in \mathbb{N}.$$

It is elementary to see that $\mathcal{I}^n_d \searrow \mathcal{C}^n$ in the sense $\mathcal{I}^n_{d+1} \subset \mathcal{I}^n_d$ for all d and $\bigcap_{d=1}^{\infty} \mathcal{I}^n_d = \mathcal{C}^n$. Yıldırım [49] refined this to his outer approximation hierarchy $\mathcal{Y}^n_d = \operatorname{Pos}(\bigcup_{k=0}^{d} \Delta^n_k)$ based on a finer grid which still has a polynomial order of cardinality in n. Since both grids are finite, the resulting approximation cones are all polyhedral, and membership of these can be tested by LP methods.

Bundfuss and Dür [10, 11] look at a hierarchy $\mathcal{H}^n = \left\{\mathcal{H}^n_d : d \in \mathbb{N}\right\}$ of nested and exhaustive simplicial partitions $\mathcal{H}^n_d$ of the standard simplex Δ^n, now employing $\operatorname{Pos}(\Delta^n) = \mathcal{C}^n$. For any fixed level $d \in \mathbb{N}$ of the hierarchy, such a partition consists of finite collection of subsimplices $\Delta \in \mathcal{H}^n_d$ such that their union gives Δ^n and their mutual intersections have zero relative volume. Each subsimplex $\Delta = \operatorname{conv}(v_1, \ldots, v_n)$ is generated by its n vertices which we collect in an $n \times n$ matrix $V_\Delta = [v_1, \ldots, v_n]$. Then it is obvious to see that $\operatorname{Pos}(\{v_1, \ldots, v_n\}) = \{S \in \mathcal{S}^n : \operatorname{diag}(V_\Delta^\top S V_\Delta) \in \mathbb{R}^n_+\}$. Even the union of all vertices of simplices in $\mathcal{H}^n_d$ is still finite, usually of cardinality polynomial in n. Thus it makes sense to define the polyhedral cone

$$\mathcal{B}^n_d = \left\{ S \in \mathcal{S}^n : \operatorname{diag}(V_\Delta^\top S V_\Delta) \in \mathbb{R}^n_+ \text{ for all } \Delta \in \mathcal{H}^n_d \right\},$$

which depends on the choice of partition hierarchy $\mathcal{H}^n$. But if this is well behaved, we have $\mathcal{B}^n_d \searrow \mathcal{C}^n$. Realizing that $\operatorname{diag} S \in \mathbb{R}^n_+$ is equivalent to $S \in \operatorname{Pos}(\mathbb{N}^n_1) \supset \mathcal{C}^n$, one is led to the following generalization in the spirit of [46]: let $\mathcal{M} \supseteq \mathcal{C}^n$ be an arbitrary outer approximation of $\mathcal{C}^n$. Then, given the partition hierarchy $\mathcal{H}^n$, define

$$\mathcal{B}_d^n(\mathcal{M}) = \{S \in \mathcal{S}^n : V_\Delta^\top S V_\Delta \in \mathcal{M}\}.$$

Bundfuss and Dür also introduced an inner approximation hierarchy: using Bezier-Bernstein representations, one quickly sees that $S \in \mathrm{Pos}(\Delta)$ if and only if $V_\Delta^\top S V_\Delta \in \mathcal{C}^n$. Of course, this equivalence cannot be used directly. Instead, the requirement $V_\Delta^\top S V_\Delta \in \mathcal{C}^n$ is relaxed by employing another (lower-level) inner approximation $V_\Delta^\top S V_\Delta \in \mathcal{M}$ for some $\mathcal{M} \subset \mathcal{C}^n$, to arrive at the inner approximation

$$\mathcal{D}_d^n(\mathcal{M}) = \left\{S \in \mathcal{S}^n : V_\Delta^\top S V_\Delta \in \mathcal{M} \text{ for all } \Delta \in \mathcal{H}_d^n\right\},$$

which again depends on the choice of partition hierarchy $\mathcal{H}^n$ but now also on the subset $\mathcal{M}$. Bundfuss and Dür originally started with $\mathcal{M} = \mathcal{N}^n$. With this choice, $\mathcal{D}_d^n(\mathcal{N}^n)$ is again a polyhedral cone, checking membership of which is of polynomial complexity in n for fixed d. Later on, Sponsel et al. [46] extended this to general $\mathcal{M}$, noting that the choice $\mathcal{M} = \mathcal{P}^n$, the psd cone, is not useful in general. Anyhow, for well-behaved partition hierarchies, we now have $\mathcal{D}_d^n(\mathcal{M}) \nearrow \mathcal{C}^n$ in the sense $\mathcal{D}_{d+1}^n(\mathcal{M}) \supset \mathcal{D}_d^n(\mathcal{M})$ for all d and $\operatorname{int} \mathcal{C}^n \subseteq \bigcup_{d=1}^{\infty} \mathcal{D}_d^n(\mathcal{M}) \subseteq \mathcal{C}^n$. It may be even worthwhile to replace the fixed class $\mathcal{M}$ by either a lower-level approximation of the same hierarchy in a recursive way, or by another inner approximation hierarchy (e.g., $\mathcal{I}_{d'}^n$, see below) for some $d' \le d$ varying with d, but to our knowledge nobody has yet explored this avenue (neither the analogous idea of $\mathcal{B}_d^n(\mathcal{M})$ which apparently is introduced here for the first time).

4.2 Parrilo's approach and sum-of-squares conditions

A different approximation approach goes back to Parrilo's thesis [40, 41] and has many contacts to semi-algebraic geometry and positive polynomials, and is therefore closely related to the Positivstellensatz [43, 45, 48], an extension of Hilbert's famous Nullstellensatz. Parrilo squared the variables $x_i^2 = y_i$ to get rid of the positivity constraint $y \in \mathbb{R}_+^n$, and arrived at a quartic

$$p_S(x) = \sum_{i,j} S_{ij} x_i^2 x_j^2 = y^\top S y.$$

Now this polynomial of degree 4 in x is for sure nowhere negative if and only if the same holds for the polynomial of degree $2(d+2)$ of the form

$$p_S^{(d)}(x) = \|x\|^{2d} p_S(x),$$

which again involves only even powers of the x_j variables. There are many sufficient conditions which guarantee $p_S^{(d)}(x) \ge 0$ for all $x \in \mathbb{R}^n$. One is that this polynomial has no negative coefficients ($\operatorname{coeff} p_S^{(d)} \ge 0$) which, again, is a condition linear in S. Another one is that $p_S^{(d)}$ can be written as a sum of squares (s.o.s.) of polynomials h_i, i.e.,

$$p_S^{(d)}(x) = \sum_i [h_i(x)]^2 \quad \text{for some polynomials } h_i.$$

The former requirement $\operatorname{coeff} p_S^{(d)} \ge 0$ gives an inner approximation hierarchy with, again, polyhedral cones. Indeed, it can be shown [4, 15] that, defining $\Theta_d^n = \left\{zz^\top - \mathrm{Diag}(z) : z \in \mathbb{N}_{d+2}^n\right\}$, we get

$$\begin{aligned}\mathcal{I}_d^n &= \left\{S \in \mathcal{S}^n : \operatorname{coeff} p_S^{(d)} \ge 0\right\}\\ &= \left\{S \in \mathcal{S}^n : \langle Z, S\rangle \ge 0 \text{ for all } Z \in \Theta_d^n\right\}.\end{aligned}$$

Again, the number of linear constraints is a polynomial in n for fixed d, so we arrive at a tractable approximation. As in [49] with $\mathcal{Y}_d^n$, one could refine this by replacing $\mathcal{I}_d^n$ with $\bigcup_{k=0}^d \mathcal{I}_k^n$ without losing polynomiality.

Returning to the s.o.s. representation $p_S^{(d)}(x) = \sum_i [h_i(x)]^2$, one can show that the polynomials h_i can be assumed to be homogeneous of degree $(d+2)$, i.e., $h_i(x) = \hat{a}_i^\top \hat{x}$ where $\hat{x} = [x^{\mathbf{m}}]_{\mathbf{m}\in\mathbb{N}_{d+2}^n}$ is the vector of all monomials $x^{\mathbf{m}} = \prod_{i=1}^n x_i^{m_i}$ of degree $d+2$ in x, and $\widehat{a_i}$ is a suitably long vector. It follows that

$$p_S^{(d)}(x) = \sum_i \left[\widehat{a_i}^\top \hat{x}\right]^2 = \hat{x}^\top M_S^{(d)} \hat{x},$$

where $M_S^{(d)}$ is a symmetric matrix of large order $r = \binom{n+d+1}{d+2}$, which obviously must be psd. Conversely, any such $M_S^{(d)} \in \mathcal{P}^r$ (the choice is not unique) gives rise to a s.o.s. representation of $p_S^{(d)}$. This matrix $M_S^{(d)}$ can be found by comparing coefficients. These conditions determine an affine subspace of matrices in $\mathcal{S}^r$, the defining constraints depend linearly on S. Thus we arrive at a linear matrix-inequality (LMI) description of this approximation hierarchy:

$$\mathcal{K}_d^n = \left\{S \in \mathcal{S}^n : M_S^{(d)} \in \mathcal{P}^r\right\} \quad \text{with } r = \binom{n+d+1}{d+2}.$$

Again it can be established [15] that $\mathcal{K}_d^n \nearrow \mathcal{C}^n$ and also $\mathcal{I}_d^n \nearrow \mathcal{C}^n$. Furthermore, $\mathcal{I}_d^n \subset \mathcal{K}_d^n$ for all d, e.g.,

$$\mathcal{I}_0^n = \mathcal{N}^n \subset \mathcal{P}^n + \mathcal{N}^n = \mathcal{K}_0^n \subseteq \mathcal{C}^n.$$

The cone $\mathcal{K}_0^n$ is often viewed as the standard zero-order approximation of $\mathcal{C}^n$. Passing to the dual cones, we arrive at the zero-order approximation(s) of $\mathcal{C}^{n*}$:

$$\mathcal{C}^{n*} \subseteq \mathcal{P}^n \cap \mathcal{N}^n = [\mathcal{K}_0^n]^* \subset \mathcal{N}^n = [\mathcal{I}_0^n]^*.$$

The dual cone $[\mathcal{K}_0^n]^*$ is often called the doubly nonnegative cone for obvious reasons.

Peña et al. [42] construct a hierarchy which has the advantage that it requires a slightly more compact LMI description: they consider

$$\mathcal{Q}_d^n = \Big\{S \in \mathcal{S}^n : (e^\top x)^d x^\top S x = \sum_{\mathbf{m}\in\mathbb{N}_d^n} x^{\mathbf{m}} x^\top Q_{\mathbf{m}} x \text{ with } Q_{\mathbf{m}} \in \mathcal{K}_0^n, \mathbf{m} \in \mathbb{N}_d^n\Big\}.$$

The right-hand side in particular includes all homogeneous polynomials with no negative coefficients (just take all $Q_{\mathbf{m}} \in \mathcal{N}^n$). So we get $\mathcal{I}_d^n \subseteq \mathcal{Q}_d^n$, and by a similar argument $\mathcal{Q}_d^n \subseteq \mathcal{Q}_{d+1}^n$. For any $S \in \mathcal{Q}_d^n$, we have $p_S^{(d)}(x) = \sum_{\mathbf{m}} x^{2\mathbf{m}} p_{Q_{\mathbf{m}}}(x)$ which obviously is a s.o.s. (recall the definition of $\mathcal{K}_0^n$), so that also $\mathcal{Q}_d^n \subseteq \mathcal{K}_d^n$ holds for all $d \in \mathbb{N}$. Hence we finally get the inclusions

$$\mathcal{I}_d^n \subseteq \mathcal{Q}_d^n \subseteq \mathcal{K}_d^n \subseteq \mathcal{C}^n$$

and therefore $\mathcal{Q}_d^n \nearrow \mathcal{C}^n$. There is also a recursive way to define $\mathcal{Q}_d^n$ (see [42]) and a tensor description of the higher-order duals $[\mathcal{Q}_d^n]^*$, and $[\mathcal{I}_d^n]^*$ was recently provided in [21]. Note that by dualization, one gets an outer approximation hierarchy for $\mathcal{C}^{n*}$ from an inner one for $\mathcal{C}^n$, and vice versa.

4.3 Lasserre's moment approach

We now turn to a third approximation approach for $\mathcal{C}^n$ using moment matrices which was introduced by Lasserre [29]. Let T be a (compact) base of $\mathbb{R}_+^n$, let μ be an arbitrary Borel measure, and f an arbitrary function defined on $\mathbb{R}_+^n$. We start with the elementary observation that $\int_T f(x)\,\mu(\mathrm{d}x) \ge 0$ if f takes no negative values over T and if the integral exists. Now suppose that

$f(x) = \sum_{\mathbf{m}\in\mathbb{N}^n_q} a_{\mathbf{m}} x^{\mathbf{m}} = \hat{a}^\top \hat{x}$ is a (homogeneous) polynomial of degree q, and that μ possesses all T-moments

$$y_{\mathbf{m}}(\mu, T) = \int_T x^{\mathbf{m}}\, \mu(\mathrm{d}x), \quad \mathbf{m} \in \mathbb{N}^n_q .$$

Then the condition

$$0 \le \int_T f(x)\, \mu(\mathrm{d}x) = \sum_{\mathbf{m}\in\mathbb{N}^n_q} y_{\mathbf{m}} \int_T x^{\mathbf{m}}\, \mu(\mathrm{d}x) = \hat{a}^\top y(\mu, T)$$

defines a half-space linear in the coefficients of f. Of course, this condition is only necessary for non-negativity of f over T. Even multiplying with positive integrable factors (assume now that $y_{\mathbf{m}}(\mu, T)$ exists for all $\mathbf{m}$), and requiring, for instance, $\int_T [g(x)]^2 f(x)\, \mu(\mathrm{d}x) \ge 0$ for all other polynomials g of degree d is, in general, only necessary for non-negativity of f over T. However, the gap between necessity and sufficiency decreases with increasing d, and in fact, vanishes if μ (and T) is chosen properly. Applying this to the quadratic form $f(x) = f_S(x) = x^\top S x$, and using $\mathrm{Pos}(T) = \mathbb{R}^n_+$, we arrive at an outer approximation hierarchy of $\mathcal{C}^n$ which can again be expressed by LMIs: first observe that for $g(x) = \sum_{\mathbf{k}\in I(d,n)} y_{\mathbf{k}} x^{\mathbf{k}}$ with $I(d, n) = \bigcup_{k=0}^{d} \mathbb{N}^n_d$ containing $s(d, n) = \binom{n+d}{d}$ elements, and defining the moment matrix

$$M_d(\mu, T) = [y_{\mathbf{k}+\mathbf{m}}(\mu, T)]_{(\mathbf{k},\mathbf{m})\in I(d,n)^2}$$

as well as $\hat{c} = [y_{\mathbf{m}}]_{\mathbf{m}\in I(d,n)}$, we see that

$$\begin{aligned}\int_T [g(x)]^2\, \mu(\mathrm{d}x) &= \sum_{\mathbf{k}\in I(d,n)} \sum_{\mathbf{m}\in I(d,n)} y_{\mathbf{k}} y_{\mathbf{m}} y_{\mathbf{k}+\mathbf{m}}(\mu, T) \\ &= \hat{c}^\top M_d(\mu, T)\, \hat{c}\,,\end{aligned}$$

which admittedly does not involve f. However, by the same reasoning we get

$$\int_T [g(x)]^2 f(x)\, \mu(\mathrm{d}x) = \hat{c}^\top M_d(f\mu, T)\, \hat{c}\,,$$

where the localizing matrix $M_d(f\mu, T)$ (think of $f\mu$ as the signed measure with Radon-Nikodym density $\frac{\mathrm{d}(f\mu)}{\mathrm{d}\mu}$ over T) is given by

$$M_d(f\mu, T) = \left[\sum_{\mathbf{n}} a_{\mathbf{n}} y_{\mathbf{k}+\mathbf{m}+\mathbf{n}}(\mu, T)\right]_{(\mathbf{k},\mathbf{m})\in I(d,n)^2} .$$

Since $M_d(f\mu, T)$ depends linearly on the coefficients of f, we end up with the LMI condition

$$0 \le \int_T [g(x)]^2 f(x)\, \mu(\mathrm{d}x) = \hat{c}^\top M_d(f\mu, T)\, \hat{c} \quad \text{for all } \hat{c} \in \mathbb{R}^{s(d,n)}$$

or equivalently $M_d(f\mu, T) \in \mathcal{P}^{s(d,n)}$. Thus we can define the class

$$\mathcal{L}^n_d(\mu, T) = \left\{S \in \mathcal{S}^n : M_d(f_S\,\mu, T) \in \mathcal{P}^{s(d,n)}\right\}.$$

Since $M_d(f\mu, T)$ is a principal submatrix of $M_{d+1}(f\mu, T)$, it is evident that $\mathcal{L}^n_{d+1}(\mu, T) \subseteq \mathcal{L}^n_d(\mu, T)$ holds for all $d \in \mathbb{N}$. Furthermore, it can be shown [29] that whenever the support of μ equals T, and if T is compact or else $T = \mathbb{R}^n_+$ and μ has not too heavy tails, i.e., satisfies Nussbaum's multivariate extension of Carleman's condition [30], then indeed $\mathcal{L}^n_d(\mu, T) \searrow \mathcal{C}^n$. All we need to implement this approximation is a closed-form expression for the moments $y_{\mathbf{m}}(\mu, T) = \int_T x^{\mathbf{m}}\, \mu(\mathrm{d}x)$. For example, for the multivariate exponential distribution μ is readily available and we have $y_{\mathbf{m}}(\mu, \mathbb{R}^n_+) = \prod_i (m_i)!$.

A related approximation hierarchy, with a focus on stable set and graph coloring problems, is constructed in [24]. Very recently, it has been observed [19] that $S \in \mathcal{C}^n$ even implies that $M_d(f_S\,\mu, T) \in \mathcal{C}^{s(d,n)*}$ for all $d \in \mathbb{N}$. Indeed, $f_S(x) \ge 0$ over $T \subseteq \mathbb{R}^n_+$ implies that

$$M_d(f_S\,\mu, T) = \int_T f_S(x)\, \hat{x}\hat{x}^\top\, \mu(\mathrm{d}x)$$

is the limit of convex combinations of rank-one matrices built upon vectors $\hat{x} \in \mathbb{R}^{s(d,n)}_+$ with entries $\hat{x}_{\mathbf{m}} = x^{\mathbf{m}} \ge 0$ as $\mathbf{m} \in I(d, n)$, since $x \in \mathbb{R}^n_+$ as the integration ranges over T. Hence, as suggested in [19], one could tighten this hierarchy by taking a tighter outer approximation, say $\mathcal{A}^{s(d,n)}_{d'} \supseteq \mathcal{C}^{s(d,n)*}$, to have a generic symbol, and refine $\mathcal{L}^n_d(\mu, T)$ to

$$\mathcal{L}^n_d(\mu, T; \mathcal{A}_{d'}) = \left\{S \in \mathcal{S}^n : M_d(f_S\,\mu, T) \in \mathcal{A}^{s(d,n)}_{d'}\right\} \subseteq \mathcal{L}^n_d(\mu, T).$$

A possible choice is $\mathcal{A}^{s(d,n)}_{d'} = [\mathcal{K}^{s(d,n)}_0]^* = \mathcal{P}^{s(d,n)} \cap \mathcal{N}^{s(d,n)}$. Also d' could vary with d. Furthermore, Dickinson and Povh looked at how different choices of μ could effect the approximation. It is also instructive to see what happens if simply $\mathcal{A}_{d'} = \mathcal{N}^{s(d,n)}$. Of course, this coarsens the hierarchy again, but depending on the choice of μ and T and possibly combining different such choices, one arrives at a new approximation hierarchy of polyhedral cones, again of a complexity polynomial in n for fixed d. However, all these approaches have yet to be explored for their practicality.

Table 1. *Summary of approximation hierarchies for the cone $\mathcal{C}^n$.*

Symbol	Mode	Method	Remarks	Ref.
$\mathcal{E}^n_d$	outer	LP	rational grid for Δ^n	[4, 15]
$\mathcal{Y}^n_d$	outer	LP	$\mathcal{Y}^n_d \subset \mathcal{E}^n_d$, grid	[49]
$\mathcal{B}^n_d$	outer	LP	simplicial partition	[10, 11]
$\mathcal{B}^n_d(\mathcal{M})$	outer	LP	$\mathcal{M} \supset \mathcal{C}^n$	new
$\mathcal{D}^n_d$	inner	LP	simplicial partition	[10, 11]
$\mathcal{D}^n_d(\mathcal{M})$	inner	LP	$\mathcal{M} \subset \mathcal{C}^{n*}$	[46]
$\mathcal{I}^n_d$	inner	LP	coeff $p^{(d)}_S \ge 0$	[40, 41]
$\mathcal{K}^n_d$	inner	LMI	$p^{(d)}_S$ is a s.o.s.	[40, 41]
$\mathcal{Q}^n_d$	inner	LMI	$\mathcal{I}^n_d \subset \mathcal{Q}^n_d \subset \mathcal{K}^n_d$	[42]
$\mathcal{L}^n_d(\mu, T)$	outer	LMI	μ-moments over T	[29]
$\mathcal{L}^n_d(\mu, T; \mathcal{A})$	outer	LMI	$\mathcal{A} \supset \mathcal{C}^{s(d,n)*}$	[19]

5 Perspectives, future research directions, and open questions

Burer's result shows that the complexity of many NP-hard discrete problems can be hidden in the copositive cone structure. The reverse problem appears to be open – for problems with simple discrete structure, is the copositive formulation solvable in polynomial time ? For instance, in the order statistics problem, where the discrete constraint reduces to $e^\top x = 1$ and all $x_i \in \{0, 1\}$, the copositive problem obtained by Burer is essentially an SDP, after adding the constraints that X is diagonal, see (6). Are there other "natural" classes of discrete problems where the corresponding copositive optimization can be solved in polynomial time? Another issue is the above addressed option to let $\mathcal{M}$, and likewise $\mathcal{A}$, vary with d and/or n in the hierarchies $\mathcal{B}^n_d(\mathcal{M})$, $\mathcal{D}^n_d(\mathcal{M})$, or likewise $\mathcal{L}^n_d(\mu, T; \mathcal{A})$. We leave these and other issues, like rational arithmetic questions for copositivity detection and related complexity issues, for future research.

Acknowledgements.. We thank Peter J. C. Dickinson for helpful comments and for providing us with a template to produce Figure 2. Samuel Burer, Volker Kaibel and Katya Scheinberg provided valuable feedback on an earlier draft of this paper.

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Discussion Column

Monique Laurent

Copositive vs. moment hierarchies for stable sets

A fundamental problem in combinatorial optimization is how to optimize a linear objective function over the $0/1$-valued points lying in a given set K or, equivalently, over the convex hull P of $K \cap \{0,1\}^n$. Typically, K is a polytope or, more generally, a semi-algebraic set defined by polynomial equations and inequalities and the goal is to find tight, tractable relaxations of P. A well-studied class of methods, from the 1990's, is 'lift-and-project', where a hierarchy $P \subseteq \cdots \subseteq K^2 \subseteq K^1 \subseteq K$ of convex relaxations is constructed, having some nice properties: Each K^t is obtained as projection of some convex set Q^t lying in higher dimension, but with the property that linear optimization over Q^t can be done in polynomial time for any *fixed* order t. Moreover, finite convergence holds: $P = K^t$ at some order t. Several constructions have been proposed, where the sets Q^t are defined by linear (lp) or by semidefinite (sdp) conditions. This includes the RLT method of Sherali and Adams, the N or N_+ operators of Lovász and Schrijver, and the most recent moment approach of Lasserre (details and references can be found in [4]). As shown in [4], it turns out that the moment hierarchy refines the other lift-and-project hierarchies.

A different approach, which has become very popular in the recent years, is copositive programming, as nicely highlighted in this Optima featured article. The starting point is to reformulate the discrete optimization problem as a linear optimization problem over the copositive cone $\mathcal{C}^n$ (or its dual) and then to approximate $\mathcal{C}^n$ by a hierarchy of lp or sdp subcones.

Here we zoom in on these two approaches based on moment theory and on copositive programming, when they are applied to the problem of computing the maximum cardinality $\alpha(G)$ of a stable (independent) set in a graph $G = (V = [n], E)$. This is one of the most basic, hard discrete optimization problems, for which the various relaxation hierarchies have been studied in great detail. Although the two approaches may seem quite different at first sight, it turns out that the moment based hierarchy also refines the copositive based hierarchy. Here we highlight these links and discuss some open questions.

Let us first start with the following classical formulation for $\alpha(G)$:

$$\alpha(G) = \max\left\{\sum_{i\in V} x_i : x_i x_j = 0 \ \forall \{i,j\} \in E,\ x \in \{0,1\}^n\right\},$$

so that the convex hull of the feasible region is the stable set polytope STAB(G). For $t \in \mathbb{N}$, $\mathcal{P}_t(V)$ denotes the collection of subsets of V with cardinality at most t. We introduce new variables $y_I = \prod_{i\in I} x_i$ for products of variables over sets $I \in \mathcal{P}_{2t}(V)$ (this is the *lift step*) and we define the *combinatorial moment matrix* $M_t(y) = (y_{I\cup J})$ indexed by $\mathcal{P}_t(V)$. Then the sdp condition $M_t(y) \succeq 0$ combined with the linear conditions $y_\emptyset = 1$, $y_{ij} = 0$ ($\{i,j\} \in E$), and $y_I \geq 0$ ($I \in \mathcal{P}_{t+1}(V)$) define a convex set Q^t, whose projection K^t gives the Lasserre moment relaxation of order t of STAB(G). Denoting by $\mathrm{las}^{(t)}(G)$ the bound obtained by optimizing the linear objective function $\sum_{i\in V} y_i$ over Q^t, we get the following hierarchy of bounds:

$$\alpha(G) \leq \mathrm{las}^{(t)}(G) \leq \cdots \leq \mathrm{las}^{(1)}(G).$$

The bound $\mathrm{las}^{(1)}(G)$ strengthens the theta number of Lovász [6] by adding nonnegativity.

Finite convergence holds: $\mathrm{las}^{(t)}(G) = \alpha(G)$ if $t \geq \alpha(G)$. This is an easy consequence of the following elementary properties of combinatorial moment matrices (Fourier analysis on the boolean cube). Let Z be the $0/1$ matrix indexed by $\mathcal{P}_n(V)$, with entry $Z_{I,J} = 1$ if $I \subseteq J$ and 0 otherwise. Its inverse has entry $(Z^{-1})_{I,J} = (-1)^{|J\setminus I|}$ if $I \subseteq J$ and 0 otherwise; Z is known as the *Zeta matrix* of the poset $\mathcal{P}_n(V)$ and Z^{-1} as its *Möbius matrix*. It is an easy exercise to verify that $M_n(y) = Z\ \mathrm{Diag}(Z^{-1}y)Z^\mathsf{T}$. This implies:

$$M_n(y) \succeq 0 \Longleftrightarrow Z^{-1}y \geq 0 \Longleftrightarrow y \in \mathbb{R}_+\{\zeta^J : J \subseteq V\};$$

here ζ^J denotes the J-th column of Z, which contains the indicator of the set J at the positions of the n singleton subsets of V. The edge conditions $y_{ij} = 0$ ($\{i,j\} \in E$) guarantee that the above decomposition of y uses only sets $J \subseteq V$ that are stable sets of G.

We now use the formulation for $\alpha(G)$ of Motzkin and Straus [7]:

$$1/\alpha(G) = \min\{x^\mathsf{T}(I_n + A_G)x : x \in \mathbb{R}^n_+, e^\mathsf{T}x = 1\}, \qquad (1)$$

where A_G is the adjacency matrix of G, e is the all-ones vector and I_n is the identity matrix. Using (1), de Klerk and Pasechnik [1] obtain the following *copositive programming* reformulation for $\alpha(G)$:

$$\alpha(G) = \min\{\lambda : \lambda(I_n + A_G) - ee^\mathsf{T} \in \mathcal{C}^n\} \qquad (2)$$

and, using conic duality, the *completely positive* reformulation:

$$\alpha(G) = \max\{\langle ee^\mathsf{T}, X\rangle : \langle I_n + A_G, X\rangle = 1,\ X \in \mathcal{C}^{n*}\}, \qquad (3)$$

where $\mathcal{C}^n$ is the cone of copositive matrices and $\mathcal{C}^{n*}$ is the dual cone of completely positive matrices.

Given a symmetric $n \times n$ matrix S and $t \in \mathbb{N}$, define the polynomial $p_S^{(t)}(x) = (\sum_{i=1}^n x_i^2)^t(\sum_{i,j=1}^n S_{ij}x_i^2x_j^2)$. Following [1, 8, 9], the cone $\mathcal{K}_t^n$ consists of the matrices S for which $p_S^{(t)}$ is a sum of squares of polynomials, $\mathcal{I}_t^n$ is the subcone of the matrices S for which all coefficients of $p_S^{(t)}$ are nonnegative, and $\mathcal{Q}_t^n$ is a cone nested between $\mathcal{I}_t^n$ and $\mathcal{K}_t^n$. By a result of Pólya [10], any strictly copositive matrix lies in some cone $\mathcal{I}_t^n$ for t large enough. Thus $\mathcal{K}_t^n, \mathcal{Q}_t^n, \mathcal{I}_t^n \nearrow \mathcal{C}^n$ as $t \to \infty$. Replacing $\mathcal{C}^n$ by $\mathcal{K}_t^n$ in (2) and $\mathcal{C}^{n*}$ by $\mathcal{K}_t^{n*}$ in (3), we obtain two semidefinite programs with the same optimum value, denoted $\vartheta^{(t)}(G)$, and the sdp hierarchy:

$$\alpha(G) \leq \vartheta^{(t)}(G) \leq \cdots \leq \vartheta^{(0)}(G)$$

of [1]. Analogously, using $\mathcal{Q}_t^n$ (resp., $\mathcal{I}_t^n$) instead of $\mathcal{K}_t^n$, we get the sdp hierarchy $\nu^{(t)}(G)$ of [9] (resp., the lp hierarchy $\zeta^{(t)}(G)$ of [1]). Thus, $\alpha(G) \leq \vartheta^{(t)}(G) \leq \nu^{(t)}(G) \leq \zeta^{(t)}(G)$ for all $t \in \mathbb{N}$.

As $\mathcal{K}_0^n = \{P + N : P \succeq 0, N \geq 0\}$, $\vartheta^{(0)}(G)$ coincides with $\mathrm{las}^{(1)}(G)$. Moreover, it is shown in [3] that the Lasserre hierarchy refines the copositive based hierarchy:

$$\mathrm{las}^{(t)}(G) \leq \vartheta^{(t-1)}(G)$$

for any $t \geq 1$. The proof relies on the dual formulation (3) and on the explicit characterization of the dual cone $\mathcal{K}_t^{n*}$ in terms of (arbitrary, non-combinatorial) moment matrices. The fact that moment matrices occur in the description of both bounds $\mathrm{las}^{(t)}(G)$ and $\vartheta^{(t-1)}(G)$ explains why it is possible to relate them. An additional ingredient in the proof is introducing the relaxation P^t of STAB(G), which consists of all vectors $x \in \mathbb{R}^n$ that can be realized as the diagonal of a matrix $X \in \mathcal{K}_t^{n*}$ satisfying $\langle A_G, X\rangle = 0$ and $X - xx^\mathsf{T} \succeq 0$. The following inequalities are shown in [3]:

$$\mathrm{las}^{(t)}(G) \leq \max_{x\in P^{t-1}} \sum_{i\in V} x_i \leq \vartheta^{(t-1)}(G).$$

It is an open question whether the inclusion $K^t \subseteq P^{t-1}$ holds between the moment and copositive based relaxations of STAB(G).

What about the convergence of the copositive based hierarchies? By Pólya's result, the lp hierarchy $\zeta^{(t)}(G)$ converges asymptotically to $\alpha(G)$. Moreover, $\alpha(G) = \lfloor \zeta^{(t)}(G) \rfloor$ for $t \geq \alpha(G)^2 - 1$ (see [1]), but finite convergence does not hold: If G is not a clique, then $\alpha(G) < \zeta^{(t)}(G)$ for all t (see [9]). For the sdp hierarchy $\vartheta^{(t)}(G)$, de Klerk and Pasechnik [1] conjecture that there is finite convergence, at the same order as for the hierarchy $\mathrm{las}^{(t)}(G)$:

Conjecture 1. [1] *$\vartheta^{(t)}(G) = \alpha(G)$ if $t \geq \alpha(G) - 1$.*

This conjecture has turned out to be surprisingly difficult. Gvozdenović and Laurent [3] can prove it for the graphs with $\alpha(G) \leq 8$, moreover they show that the result still holds for the weaker sdp hierarchy $\nu^{(t)}(G)$ (extending results of [1, 9]). The technical details for this partial convergence result are however considerably more involved than the convergence result for $\mathrm{las}^{(t)}(G)$.

Why is the parameter $\mathrm{las}^{(t)}(G)$ much easier to handle than the parameter $\vartheta^{(t)}(G)$? A reason might lie in the fact that the formulation of the former bound incorporates in an explicit manner the integrality $0/1$ condition on the variables, while the latter bound does not. Another reason lies in the cone $\mathcal{K}_t^n$ which appears to be quite difficult to work with. For instance, for $t \geq 1$, it is not invariant under some simple matrix operations like adding a zero row and column to a matrix, or scaling by pre- and post-multiplying by a positive diagonal matrix (two operations which obviously preserve copositivity and positive semidefiniteness). Here is another related open question.

Conjecture 2. [3] *If u is an isolated node of G then, for all $t \geq 0$, $\vartheta^{(t)}(G) \leq \vartheta^{(t)}(G \setminus u) + 1$.*

It is shown in [3] that Conjecture 2 implies Conjecture 1. It is thus interesting to note that the conjectured convergence result for the hierachy $\vartheta^{(t)}(G)$ is closely related to the behavior of the parameter $\vartheta^{(t)}(G)$ under the simple graph operation of deleting isolated nodes.

As briefly discussed here, the copositive programming approach raises interesting open questions already for the well-studied maximum stable set problem. Many other aspects of copositive programming are currently in the focus of attention, leading to fascinating research questions. For example, the *cp-rank* of completely positive matrices is closely related to the notion of *nonnegative rank* which in turn ties to fundamental questions about the extension complexity of polytopes, as shown in the seminal work of Yannakakis [11]. Going back to our starting point, lift-and-project methods aim to represent a given $0/1$ polytope P as projection of some higher dimensional, hopefully nicer, convex set Q. The smallest number of facets that such a polytope Q can have is (roughly) the *extension complexity* of P. The recent breakthrough result of [2] shows exponential extension complexity for the stable set polytope, the cut polytope and the TSP polytope. This settles a long-standing open question of [11] and rules out the existence of compact linear programming extended formulations for these problems. The analogous question of existence of compact *semidefinite programming* extended formulations remains open.

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Charles Broyden Prize

The Charles Broyden Prize for the best paper published in the journal Optimization Methods and Software in 2011 is awarded to Didier Henrion and Jerome Malick for the paper *Projection Methods for conic feasibility problems, applications to polynomial sum-of-squares decompositions* published in Volume 26, No. 1, pp. 23–46.

This article will be freely available until the end of 2012 at http://www.tandfonline.com/doi/pdf/10.1080/10556780903191165. The paper was unanimously chosen by the prize committee, and in their opinion represents an excellent contribution to the optimization literature.

Michael Ferris (Chair), Frederic Bonnans, Masao Fukushima, Nickolaos Sahinidis, Yinyu Ye (Prize Committee)

Call for Nomination/Submission Best Paper Prize for Young Researchers in Continuous Optimization

Fourth Mathematical Optimization Society International Conference on Continuous Optimization, ICCOPT 2013 (Universidade Nova de Lisboa, Lisbon, Portugal, July 27 – August 1, 2013)

Nominations/Submissions are invited for the Best Paper Prize by a Young Researcher in Continuous Optimization.

The submitted papers should be in the area of continuous optimization and satisfy one of the following three criteria:

(a) Passed the first round of a normal refereeing process in a journal;
(b) published during the year of 2010 or after (including forthcoming);
(c) certified by a thesis advisor or postdoctoral mentor as a well-polished paper that is ready for submission to a journal.

Papers can be single-authored or multi-authored, subject to the following criterion:

(d) Each paper must have at least one qualifying author who was under age 30 on January 1, 2008 and has not earned a Ph.D before that date. In case of joint authorship involving senior researchers (i.e., those who fail both the age test and the Ph.D. test), one senior author must certify the pivotal role and the relevance of the contribution of the qualifying author in the work. The Selection Committee will decide on questions on eligibility in exceptional cases.

The selection criteria will be based solely on the quality of the paper, including originality of results and potential impact.

The following items are required for submission:

A. The paper for consideration;
B. a brief description of the contribution (limited to 2 pages)
C. a statement about the status of the paper: not submitted, under review, accepted, or published (when) in a journal;
D. a certification of the qualifying author's eligibility in terms of age and Ph.D. (by the qualifying author's advisor or department chair);

E. in case of joint authorship involving a senior researcher, a certification by the latter individual about the qualifying author's pivotal role and relevance of the contribution.

The deadline for submission is April 1, 2013. Submission should be sent electronically in Adobe Acrobat pdf format, to the Chair of the Selection Committee, Professor Stefan Ulbrich, email address: ulbrich@mathematik.tu-darmstadt.de.

Up to three papers will be selected as finalists of the competition. The finalists will be featured in a dedicated session at ICCOPT 2013, and the Prize Winner will be determined after the finalists session. The Young Researcher Prize in Continuous Optimization will be presented at the conference banquet. The finalists will receive free registration to ICCOPT 2013 and to the conference banquet. Their university or department should cover the travel costs. All the three finalist will receive a diploma, and the winner will be presented a $1000 USD award.

Selection Committee: Sam Burer (samuel-burer@uiowa.edu)
Jean-Baptiste Hiriart-Urruty
(jean-baptiste.hiriart-urruty@math.univ-toulouse.fr)
Stefan Ulbrich (Chair) (ulbrich@mathematik.tu-darmstadt.de)

Optimization Methods and Software (OMS): Special Issue in Honor of Prof. Florian Potra's 60th birthday

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Polynomial Optimisation 2013 Isaac Newton Institute for Mathematical Sciences July 15 to August 9

Optimisation problems involving polynomials arise in a wide variety of contexts, including operational research, statistics, probability, finance, computer science, structural engineering, statistical physics, combinatorial chemistry, computational biology and algorithmic graph theory. They are however extremely challenging to solve, both in theory and practice. Existing algorithms and software are capable of solving only very small instances to proven optimality, unless they have some amenable structure, such as sparsity or convexity.

A fascinating feature of polynomial optimisation is that it can be approached from several different directions. In addition to traditional techniques drawn from operational research, computer science and numerical analysis, new techniques have recently emerged based on concepts taken from algebraic geometry, commutative algebra and moment theory. In this regard, polynomial optimisation provides a valuable opportunity for researchers from previously unrelated disciplines to work together.

The plan for this four-week programme is as follows. During the first week (15th – 19th July 2013), there will be a "summer school" and a "workshop". The "summer school" will consist of a series of tutorials from internationally respected invited speakers, and the workshop will consist of a series of contributed talks and possibly a poster session. These events will be open not only to official programme participants, but also to other interested academics, PhD students and post-doctoral researchers (space permitting).

The following three weeks will be open only to invited persons. Each of the three weeks will focus on a specific sub-topic:

1. Algebraic Approaches (July 22–26, 2013). This will concern the development of new theory and algorithms based on techniques from relevant areas of pure mathematics, such as real algebraic geometry, commutative and noncommutative algebra, moment theory and the theory of sums-of-squares representations.
2. Convex Relaxations and Approximations (July 29 – August 2). This will be devoted to the study of convex relaxations (and hierarchies of relaxations) of certain important specially-structured problem classes, along with associated approximation algorithms (and inapproximability results).
3. Algorithms and Software (August 5–9). This will be devoted to the development of new algorithms and their implementation as software. This may include, for example, algorithms for computing lower and upper bounds, algorithms for generating strong valid inequalities, and algorithms for solving instances to proven optimality.

Organisers: Joerg Fliege (Southampton), Jean-Bernard Lasserre (Toulouse), Adam Letchford (Lancaster), Marcus Schweighofer (Konstanz)
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ICCOPT 2013

The Fourth International Conference on Continuous Optimization, will take place in Lisbon, Portugal, from July 27 to August 1, 2013. ICCOPT is a recognized forum of discussion and exchange of ideas for researchers and practitioners in continuous optimization, and one of the flagship conferences of the Mathematical Optimization Society.

ICCOPT 2013 is organized by the Department of Mathematics of FCT, Universidade Nova de Lisboa, in its Campus de Caparica, located near a long beach, 15 minutes away by car (and 30 by public transportation) from the center of Lisbon, on the opposite side of the river Tagus.

ICCOPT 2013 includes a Conference and a Summer School. The Conference (July 29 – August 1) will count with the following Plenary Speakers:

- Paul I. Barton (MIT, Massachusetts Inst. Tech.)
- Michael C. Ferris (Univ. Wisconsin)
- Yurii Nesterov (Univ. Catholique de Louvain)
- Yinyu Ye (Stanford Univ.)

and the following Semi-plenary Speakers:

- Amir Beck (Technion, Israel Inst. Tech.)
- Regina Burachik (Univ. South Australia)
- Sam Burer (Univ. Iowa)
- Coralia Cartis (Univ. Edinburgh)
- Michel De Lara (Univ. Paris-Est)
- Victor DeMiguel (London Business School)
- Michael Hintermüller (Humboldt-Univ. Berlin)
- Ya-xiang Yuan (Chinese Academy of Sciences)

The Summer School (July 27–28) is directed to graduate students and young researchers in the field of continuous optimization, and includes two courses:

– Summer Course on PDE-Constrained Optimization (July 27, 2013), by
  - Michael Ulbrich (Tech. Univ. Munich)
  - Christian Meyer (Tech. Univ. Dortmund)

– Summer Course on Sparse Optimization and Applications to Information Processing (July 28, 2013), by
  - Mário A. T. Figueiredo (Technical Univ. Lisbon and IT)
  - Stephen J. Wright (Univ. Wisconsin)

There will be a paper competition for young researchers in Continuous Optimization (see Page 10 of this issue; further information available from the website below).

The three previous versions of ICCOPT were organized respectively in 2004 at Rensselaer Polytechnic Institute (Troy, NY, USA), in 2007 at McMaster University (Hamilton, Ontario, Canada), and in 2010 at University of Chile (FCFM, Santiago, Chile).

The meeting is chaired by Luis Nunes Vicente (Organizing Committee) and Katya Scheinberg (Program Committee) and locally coordinated by Paula Amaral (Local Organizing Committee).

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