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## Mixed-integer Nonlinear Optimization: A Hatchery for Modern Mathematics

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**ABSTRACT.** The aim of this workshop was fostering the growth of new mathematical ideas arising from mixed-integer nonlinear optimization. In this regard, the workshop has been a resounding success. It has covered a very diverse scientific landscape, including automated proof in computational geometry, the analysis of computational complexity of MINO in fixed and variable dimension, the solution of infinite MINO such as those appearing in mixed-integer optimal control, the theoretical and computational deployment of traditional integer and continuous approaches to achieve new solution algorithms for large-scale MINO, a classification of the most interesting engineering and technology applications of MINO, and more. It has synthesized twenty open questions and challenges which will serve as a roadmap for the years to come.

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### Introduction by the Organisers

Mixed-Integer Nonlinear Optimization (MINO) is a subfield of Mathematical Optimization (MO) which studies formulations involving both integer and continuous variables, as well as linear and nonlinear functions on these variables, and the methods used to find their solutions.

**Definition.** MINO can be seen as a formal language used to describe a very large class of optimization problems. Each valid sentence of this language is called a *formulation*. Formulations consist of decision variables, parameters, objectives

and constraints, and are written as follows:

$$(1) \quad \left. \begin{array}{l} \min \quad f(x, p) \\ \forall i \in I \quad g_i(x, p) \leq 0 \\ \forall j \in Z \quad x_j \in \mathbb{Z}, \end{array} \right\}$$

where  $I, Z$  are index sets. The parameter vector  $p$  lists elements from a number field (e.g.  $\mathbb{Q}$ ), and encodes the input of the problem (also called *instance*). The decision variable vector  $x$  is a list of variable symbols; it encodes the output of the problem (also called the *solution*). The function symbols  $f, g_i$  (for each  $i \in I$ ) are valid sentences of another formal language having  $x_1, x_2, \dots$  and elements of  $\mathbb{Q}$  as atoms, which can be recursively combined using arithmetic operators (including powers) and a few transcendental functions such as  $\log, \exp$  and so on. The last constraint in Eq. (1) expresses an integrality requirement on the variables indexed in  $Z$  (the other variables are assumed to be continuous).

**Motivation.** The interest of expressing optimization problems formally by means of MO formulations such as Eq. (1) is that there are solution methods which address all instances in a certain class. Specifically, one can solve Eq. (1), at least in practice, using a range of rather powerful *solver* algorithms, such as spatial Branch-and-Bound. This shifts the focus from designing and implementing algorithms for solving problems (which is hard) to modelling an application using the formal language (which is easier). All sorts of problems arising in industry, science, technology can be modelled as MINO, but there are many possible MINO representations of a given optimization problem, and not all of them yield the same solver performance. A crucial problem is then that of *reformulation*, which aims at finding MINO representations which are good from the point of view of the solver (see e.g. J.P. Vielma's talk). In particular, humans model using quantifiers over index sets in order to express properties of indexed variables and indexed parameters, whereas solvers require unquantified input. Quantified formulations are also called *structured*, whereas the solver input format is known as *flat*.

**Organization.** The workshop consisted of five tutorial-type talks (45' followed by 15' discussion), twenty invited talks (30' followed by 15' discussion), and eighteen short research announcements (10' followed by 5' discussion). We also organized two optional sessions: one on open problems and challenges, and a second one about the mathematically-oriented computer language Julia, with its mathematical programming extension JuMP. Among the most interesting open problems, we emphasize a stress on extended formulation size and complexity, verification of copositivity and complete positivity, the solution of a variety of small, but very hard, mostly geometrical MINO problems, automatically recognizing some structural features of a given formulation, finding tight convex relaxations of nonconvex functions that are hard to optimize, dealing with black-box nondifferentiable functions.

Each day started with one of the tutorial talks, then continued with a variety of invited talks focusing mainly on the pillars of our *hatchery for modern mathematics*: hierarchies of approximations, mixed-integer nonlinear optimal control,

the power of lifting, big data. On tuesday we scheduled an afternoon session with six research announcements, and on thursday we had nine. Wednesday afternoon saw the traditional hike, and friday was a full working day.

**Topics of the tutorial talks.** Mixed-integer control problems, such as those arising in the control of chemical plants or automatic vehicles, are among the most difficult in the MINO arena, due to their potentially large size, the range of nonlinearities which appear in the problem function forms, and the fact that the constraints are often differential equations and/or nondifferentiable “black-box” functions (see e.g. Armin Fügenschuh’s and the Simons fellow Sven Leyffer’s talks).

Currently, one of the topics which draws the most attention is solving polynomial MINO problems, ranging from quadratic (see e.g. A. Del Pia’s talk) to general polynomial. In the latter case, Semidefinite Programming (SDP) formulations are often employed — these are MO formulations involving positive semidefiniteness of a certain matrix involving some decision variable symbols (see A.A. Ahmadi’s talk). More precisely, the most promising approach to provide valid bounds are relaxation hierarchies, such as Lasserre’s (who was part of the audience at the workshop — also see E. De Klerk’s talk).

Interestingly for mathematics, MINO type problems can also be used to derive proofs. Specifically, many geometrical problems can be cast as MINO; there exist various techniques for turning such solutions into proofs, as shown by some of the speakers at this workshop (e.g. F. Vallentin’s talk).

Finally, the current trend emphasizing the availability of increasingly large amounts of data from security, retail, social networking and other sources suggests the possibility of finding relationships between many data sources, and exploit them in a concerted or integrated way. This presents the enormous difficulty of having to not only solve enormous optimization problems, but also that of leveraging the data to actually yield, or at least validate, the formulation (see A. Lodi’s talk).

**The short research announcements.** We cover SRAs here since they are not included in the abstracts below.

J. Linderoth presented *GüBoLi*, a new solver for nonconvex box-constrained quadratic programs using Integer Programming (IP) software technology. L. Hupp discussed IP approaches for structured binary quadratic optimization problems, with special attention to quadratic matching. S. Sorgatz presented results on improving the flow of vehicular traffic at traffic light intersections. R. Misener presented a technique for automatically recognizing pooling problem structure in arbitrary flat MINO problems. S. Onn talked about lexicographical combinatorial optimization. M. Firsching, who was not part of our workshop but was working on the editorial board of MFO’s *snapshot program*, presented a technique for turning floating point solutions of MINO problems into minimal polynomials of the correct algebraic number. F. Liers provided a structural investigation of piecewise linearized network flow problems. K. Anstreicher proved that the SDP relaxation of quadratic optimization with ellipsoidal hollows is exact if the SDP

relaxation of the same problem without hollows is exact. S. Wiese studied indicator constraints in the linear job-shop scheduling problem. L. Mencarelli presented a multiplicative weights update algorithm for MINO problems. Ky Vu introduced a new randomized algorithm for restricted linear membership problems based on random projections. A. Gupte discussed explicit disjunctive inequalities for some structured nonconvex sets. S. Dey presented new formulations and valid inequalities for the AC optimal power flow problem. S. Weltge discussed the size of SDP extensions. A. Martin's talk was about an ongoing effort within a large grant for network problems including physical transport. P. Belotti discussed the impact of the presolver in solution algorithms for MINO problems. Finally, P. Bonami gave a talk about solving empty mixed integer second-order conic programs (MISOCP) using the CPLEX solver.

**A need.** One of the most senior members of the MINO community, I. Grossmann, expressed a need for developing a conceptual roadmap showing the interconnections of all the theoretical subproblems that are being addressed by the various MINO researchers. This should ultimately lead to better solutions of general MINO and mixed-integer nonlinear control problems. This accomplishment would provide the MINO field with a stronger theoretical foundation.

**The future.** In view of the very stimulating interaction between the researchers during the workshop and of the presumably ongoing strong interest in symmetries in optimization problems (as demonstrated by the many open directions of future research), the workshop participants strongly agreed that a similar meeting in two years would be most desirable. We are exploring various possibilities with other mathematical centers such as CIRM in Marseille, Cargèse in Corsica, Bertinoro in Italy, and so on. The idea of submitting another application to the MFO in three or four years was received enthusiastically, and encouraged by the Director of the MFO.

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## Workshop: Mixed-integer Nonlinear Optimization: A Hatchery for Modern Mathematics

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## Abstracts

### Open problems

SVEN LEYFFER (CHAIR)

The presentation of the open problems follows the same order of presentation as at the workshop.

- (1) [*Linderoth*] Why is Semidefinite Programming (SDP) so slow?
- (2) [*Linderoth*] Let  $X(\alpha, \beta, \gamma) = \{(x_1, x_2, t_1, t_2, z_1, z_2) \in \mathbb{R}^4 \times \{0, 1\}^2 \mid t_1 \geq x_1^2 \wedge t_2 \geq x_2^2 \wedge 0 \leq \alpha x_1 + \beta x_2 \leq z_1 \wedge 0 \leq \gamma x_2 \leq z_2\}$ , with  $\alpha, \gamma$ . What is a compact description of  $\text{conv}(X(\alpha, \beta, \gamma))$  which can be scaled up to arbitrary sizes?
- (3) [*Vielma*] Mathematical programming feasible sets having non-semialgebraic (non-representable as a finite number of polynomial inequalities) convex hull: what is the minimum number of additional variables required for representing the convex hull as semialgebraic sets?
- (4) [*Liberti*] Randomized algorithms for determining copositivity ( $\forall x \geq 0 \ x^\top A x \geq 0$ ) and complete positivity ( $A = BB^\top$  for some nonnegative  $n \times k$  matrix  $B$ ) of a matrix.
- (5) [*Liberti*] Recognizing named structures in a given (flat) Mathematical Program (MP). Here I am seeing MP as a formal language for expressing mathematical optimization problems; its expressions and constraints can be either *structured* (if they involve sum/product or universal quantifiers  $\sum, \prod, \forall$ ) or *flat* (otherwise). Humans write MPs in structured form, but solvers need flat MPs as input. The translation is usually carried out by a modelling environment. A “named structure” is simply a label, such as ASSIGNMENT, FLOW, POOLING (etc.) which describes a well-known MP. Named structures will be typically parametrized, e.g. a FLOW will be described by a possibly weighted digraph  $G$ , perhaps a set of source ( $S$ ) and target ( $T$ ) vertices, as well as the decision variables used ( $x$ ), so as to appear as FLOW( $G, S, T, x$ ). A formalization of this problem can probably be attained by specifying a finite list of named structures to be recognized, together with a grammar for their recognition within the MP language.
- (6) [*Anstreicher*] “Most outstanding open problem in global optimization”: example in dimension  $n = 3$ . Take the dodecahedron circumscribing the sphere of radius 1, and let  $R$  be the radius of the sphere circumscribing the dodecahedron. Sample  $m \geq 12$  points in the spherical shell  $[1, R]$  that are all at least distance one from one another. **Claim:**  $\sum_{i \leq m} \|x_i\|_2 \geq 12 + (m - 12)R$ . Thomas Hales claims to have proved it in his book, but the proof is unwieldy. There are “good” proofs for  $m \leq 16$ . Find “good” proofs for  $m > 16$ . (See Anstreicher’s paper.)
- (7) [*Dey*] Same as Anstreicher’s but with  $\|\cdot\|_1$  norm. (Named the “Leon” problem)

- (8) [Ahmadi] Find a convex nonnegative polynomial which is not Sum Of Squares (SOS). Motivation: if you want to minimize a polynomial function  $p(x)$ , unconstrained, you can reformulate this as  $\gamma = \max \gamma$  s.t.  $p(x) - \gamma$  is SOS. In general, we have  $\gamma \leq \gamma^* = \min p(x)$ . There are  $p$ 's yielding  $<$  but not convex. Any good polynomial must be convex but not SOS-convex (i.e. the Hessian must not factor) — this is a necessary but not sufficient condition. A good candidate is like Motzkin's polynomial, but convex. Techniques based on optimizing directions in polynomial coefficient space.
- (9) [Ahmadi] Let  $P_{n,d} = \{p(x) \in \mathbb{R}^d[x] \mid \forall x \in \mathbb{R}^n p(x) \geq 0\}$ , which is a convex set. Let  $\Sigma_{n,d} = \{p(x) \mid p = \sum_i q_i^2(x)\}$ , which is convex. Are the intermediate sets  $\Sigma_{n,d}^k = \{p(x) \mid \exists q \in \mathbb{R}^k[x] (q\text{SOS} \wedge pq\text{SOS})\}$  also convex?
- (10) [Onn] Given finite sets  $S_0, \dots, S_d \subset \mathbb{R}^d$  such that 0 is contained in the convex hull of each  $S_i$ , there is a theorem which states that there is an  $s_i \in S_i$  such that  $0 \in \text{conv}\{s_0, \dots, s_d\}$ . What is the complexity of finding such  $s_i$ 's? (The version where  $S_i = S_j$  is Carathéodory's theorem. See Barany and Onn, MOR 1997. Also see Antoine Deza's "Colorful Linear Programming" web page.)
- (11) [Dey] Take an ILP feasible set  $F = \{x \in \mathbb{Z}^n \mid Ax \leq b\}$  and a fractional point  $x^*$  in the relaxation  $\bar{F}$  of  $F$ . Determine  $\alpha \in \mathbb{Z}^n$  and  $\beta \in \mathbb{R}$  such that  $\alpha x \leq \lfloor \beta \rfloor$  is valid for  $F$  but violated by  $x^*$ . What is the complexity of this problem? Note it is unknown also if  $Ax \leq b$  consists of one row only.
- (12) [Dey]  $\min x^\top Ax + b^\top x$  s.t.  $x \in P \cap \mathbb{Z}^n$  where  $P$  is a rational polytope. This problem is polytime when  $n = 2$ . What's the complexity when  $n = 3$ ?
- (13) [Misener] Practical rules for knowing when to apply SDP and RLT cuts together.
- (14) [Leyffer] Given  $\min f(x)$  s.t.  $x \in X \subset \mathbb{Z}^p \times \mathbb{R}^q$ . Given  $f$  as an evaluation oracle on integer points only. What's a practical algorithm for solving this problem?
- (15) [Dey-Averkov] Is the convex hull of a (polyhedron set difference a finite number of other polyhedra) polyhedral?
- (16) [Grossmann] Convexification of several major classes of convex mixed-integer programming problems in the spirit of convexification of 0-1 MILP problems (eg Lovasz & Schrijver (1989), Sherali & Adams (1990), Balas, Ceria, Cornuejols (1993)) that yield the true convex hull with which the mixed-integer program can theoretically be replaced by a continuous optimization problem that yields the same solution as the original MILP model. The transformation will of course be exponential but might lead to a basis for deriving cutting planes as was done in MILP (e.g. lift and project). The classes of convex mixed-integer programming problems could comprise from general convex to specialized like convex MIQP. Furthermore, the above should include the case of bounded integers as opposed to only 0-1s.
- (17) [Grossmann] Establishing theoretical sufficient conditions under which a 0-1 optimal control problem leads to a convex relaxation. Furthermore,

determine whether it is possible to convexify such a problem so that it will yield the true convex hull as in the above.

- (18) [*Grossmann*] Determine whether the nonconvex binary quadratic program can be replaced by an equivalent convex continuous program even if it requires an exponential transformation.
- (19) [*Grossmann*] Determine whether for a nonconvex MINLP (including special cases like MIQP) one can determine what is the "optimal" lower bound that can be predicted for the convex relaxation irrespective of what specific method one uses.
- (20) [*Grossmann*] What is the most general modeling formulation that one can use for discrete/continuous optimization models (e.g. algebraic MINLP, GDP or another for both 0-1 and general integer)?

### **LP and SOCP-based algebraic techniques for nonlinear and integer optimization**

AMIR ALI AHMADI

(joint work with Anirudha Majumdar)

In recent years, algebraic techniques in optimization such as sum of squares (SOS) programming have led to powerful semidefinite programming relaxations for a wide range of NP-hard problems in computational mathematics. While the continuous optimization community has championed these tools in various application domains (e.g., polynomial optimization, dynamics and control, robotics), the reception from the integer programming (IP) community has not been as strong. The primary reason for this, we suspect, is scalability: while SOS techniques are known to produce strong semidefinite relaxations, the IP community tends to prefer weaker but cheaper relaxations based on linear programming that can be made stronger for example through iterative application in a branch-and-bound scheme.

In this work, we introduce new algebraic relaxation schemes that are very similar to SOS relaxations in nature but instead of semidefinite programs result in linear or second order cone programs. These are what we call "DSOS and SDSOS programs." We show that these relaxations are orders of magnitude more scalable than SOS relaxations while enjoying many of the same asymptotic theoretical guarantees. The new tools have the potential for providing fast and competitive lower bounds on mixed-integer (nonlinear) programs, especially if implemented in branch and bound schemes.

At a high level, our idea is to replace the positive semidefiniteness constraint on the Gram matrices that appear in SOS programs with the more restrictive constraints that they be *diagonally dominant* or *scaled diagonally dominant*. These new conditions can respectively be imposed with linear programming and second order cone programming.

We use this simple idea as the basis of several hierarchies that inner approximate the cone of positive semidefinite matrices with increasing accuracy. It is shown that

the new hierarchies (which consist of solving linear or second order cone programs only) can solve arbitrary polynomial optimization problems to arbitrary accuracy.

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### Constructive Approaches to Positivstellensätze

GENNADIY AVERKOV

Positivstellensätze are results characterizing a polynomial  $f$ , strictly positive on a semialgebraic set  $S$ , in terms of a representation for  $f$  that provides the ‘algebraic evidence’ of the positivity of  $f$  on  $S$ . One can distinguish two types of positivstellensätze: those in which the representation for  $f$  involves fractions of polynomials (positivstellensätze with denominators) and those with the representation for  $f$  involving multiplication and addition of polynomials only (denominator-free positivstellensätze). Denominator-free positivstellensätze are of particular interest in polynomial optimization since they can be used to develop (approximate) methods of solving polynomial optimization problems. The best-known denominator-free positivstellensätze are due to Schmüdgen [1] and Putinar [2]; they deal with an arbitrary nonempty and bounded subset  $S$  of  $\mathbb{R}^d$  defined by a system of non-strict polynomial inequalities. Furthermore, the positivstellensätze of Handelman [3] and Jacobi & Prestel [4] deal with the interesting special case of  $S$  being a polytope. We abbreviate the mentioned results of Jacobi & Prestel, Handelman, Putinar and Schmüdgen by (JP), (H), (P) and (S), respectively. The highly non-constructive original proofs of (JP), (H), (P) and (S) employ nontrivial algebraic and/or functional analytic arguments. In the last decades, several authors suggested alternative proofs of (JP), (H), (P) and (S). A short algebraic proof of (S), which uses the representation theorem for real commutative rings<sup>1</sup> and the Positivstellensatz of Krivine [9] and Stengle [11], was given by Berr & Wörmann [12]. Later, Schweighofer [13] modified the argument of Berr & Wörmann to give a more elementary proof of (S), which does not employ the above mentioned representation theorem. In the same publication Schweighofer also gave a short constructive proof of (H), based on Pólya’s theorem [14] and Hilbert’s Basis Theorem (see also Powers & Reznick [15]). Furthermore, Schweighofer [16] gave a constructive proof of (JP) and a special case of (P).

We show that the approach developed by Berr & Wörmann and Schweighofer can be used to give a unified and short proofs of (JP), (H), (P) and (S). One of the aims of the manuscript is to present these denominator-free positivstellensätze

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<sup>1</sup>This representation theorem is usually attributed to Kadison [5] and Dubois [6], though as pointed out by Marshall [7] and Prestel [8] it was proved before Dubois by Krivine [9, 10].

altogether in a self-contained form accessible to non-experts. The presented proofs of (JP) and (H) are constructive and elementary. In contrast to the proof of Schweighofer, our proof of (H) does not employ Hilbert's Basis Theorem. All currently known proofs of (P) and (S), including the proofs presented here, use the positivstellensatz of Krivine and Stengle and thus depend on non-elementary tools from real algebraic geometry, such as Tarski's Transfer Principle.

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### The theta number of abstract simplicial complexes

CHRISTINE BACHOC

(joint work with Anna Gundert, Alberto Passuello and Alain Thiery)

Many classical problems in mathematics can be restated as the determination of the independence number of a graph or of a hypergraph. In most cases, this is a difficult task, and therefore convex approximations in the form of semidefinite programs are often used instead of an exact value.

For a graph  $G = (V, E)$ , its theta number  $\vartheta(G)$ , introduced by Lovász in [7], gives an upper bound of its independence number  $\alpha(G)$ . Starting from  $\vartheta(G)$ , better and better approximations can be obtained through one of many available semidefinite programming hierarchies. The most commonly used arises from Lasserre hierarchy for polynomial optimization problems [4], [5]; moreover Lasserre formulation also applies to upper approximate the independence number of a hypergraph.

These approaches have lead to remarkable numerical results see e.g. [8]; however, when the issue is to provide upper bounds in closed form for parametrized families of graphs, or to obtain information on the asymptotic behavior of the independence number when some parameters go to infinity like in [6] or [2], the featured method is much more crude and mainly relies on earlier inequalities due to Hoffman and Delsarte. Hoffman bound applies to a  $d$ -regular graph with adjacency matrix  $A_G$ :

$$(1) \quad \alpha(G) \leq \frac{-n\lambda_{\min}(A_G)}{d - \lambda_{\min}(A_G)}$$

where  $\lambda_{\min}(A_G)$  stands for the smallest eigenvalue of  $A_G$ . Delsarte bound [1] is a generalization of Hoffman bound. A matrix  $A$  is said to be a pseudo-adjacency matrix of a graph  $G$  if  $A_{ij} = 0$  when  $\{i, j\}$  is not an edge of  $G$  and if the all-one vector is an eigenvector of  $A$  with associated eigenvalue  $\lambda_1 > 0$ . Then

$$(2) \quad \alpha(G) \leq \frac{-n\lambda_{\min}(A)}{\lambda_1 - \lambda_{\min}(A)}.$$

It can be easily seen that these two bounds are immediate consequences of the inequality  $\alpha(G) \leq \vartheta(G)$ .

In this talk, we consider the case of a uniform hypergraph  $\mathcal{H}$  on the vertex set  $V$ , with set of hyperedges  $\mathcal{E}$ , each hyperedge being an element of  $\binom{V}{k+1}$ . Its independence number is by definition the maximal cardinal of a subset of vertices that does not contain any hyperedge. We identify  $\mathcal{H}$  with the abstract simplicial complex  $X$  of dimension  $k$  with complete  $(k-1)$ -skeleton and with set of  $k$ -dimensional faces  $X_k = \mathcal{E}$  (we recall that an abstract simplicial complex on  $V$  is simply a collection of subsets of  $V$  called faces, such that the subsets of a face are also faces, and that the dimension of a face is one less than its cardinal). In this framework, we define a natural analog of the theta number, denoted  $\vartheta_k(X)$ , which is an upper bound for the independence number of  $X$ . We derive an analog of Hoffman inequality for regular simplicial complexes, that involves the adjacency matrix of the simplicial complex (see [3]), and an analog of Delsarte inequality for a suitable notion of pseudo-adjacency matrices of a simplicial complex.

Moreover, we build in a similar way a complete hierarchy, i.e. a sequence  $\hat{\vartheta}_\ell(X)$ ,  $k \leq \ell \leq \alpha(X)$ , of decreasing values, starting with  $\vartheta_k(X)$ , and ending at  $\hat{\vartheta}_{\alpha(X)}(X) = \alpha(X)$ , each of them thus providing a semidefinite programming upper bound for  $\alpha(X)$ .

Finally, we analyze  $\vartheta_k(X)$  when  $X = X^k(n, p)$  is the random  $k$ -complex in the model of Linial and Meshulam. In the range  $c_0 \log(n)/n \leq p \leq 1 - c_0 \log(n)/n$ , we

show that  $\vartheta_k(X^k(n, p)) = \Theta(\sqrt{(n-k)q/p})$ , where  $q = 1 - p$ , therefore extending to simplicial complexes a well-known result for random graphs.

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## Combinatorial Optimal Control of Semilinear Elliptic PDEs

CHRISTOPH BUCHHEIM

(joint work with Christian Meyer and Renke Schäfer)

Mixed-integer optimal control problems (MIOCP) are often addressed by first discretizing the differential equations and then applying standard software for solving the resulting mixed-integer nonlinear programs (MINLP). Usually, due to their size, the discretized problems can be solved to proven optimality only in small dimension, in particular in the non-convex case. For this reason, most literature about mixed-integer optimization under partial differential equation (PDE) constraints only deals with linear PDEs.

We consider nonlinear elliptic PDEs with a convex nonlinear part instead, concentrating on combinatorial optimal control problems of the form

$$\begin{aligned}
 & \min \quad c^\top u \\
 & \text{s.t.} \quad y(x) \geq y_{\min}(x) \quad \text{a.e. in } \Omega \\
 \text{(COCP)} \quad & Ay + g(y) = \sum_{i=1}^{\ell} u_i \psi_i \quad \text{in } \Omega \\
 & \frac{\partial y}{\partial n_A} + b(y) = \sum_{j=\ell+1}^n u_j \phi_j \quad \text{on } \Gamma_N \\
 & y = 0 \quad \text{on } \Gamma_D \\
 & \text{and } u \in \mathcal{U}.
 \end{aligned}$$

Here we assume that  $\mathcal{U} \subseteq \mathbb{Z}^n$  is a set of discrete controls given by an integer linear description. In particular, we can model general combinatorial constraints on the control vector  $u$ . The domain  $\Omega \subset \mathbb{R}^d$ ,  $d \in \mathbb{N}$ , is bounded with  $\partial\Omega = \Gamma_D \cup \Gamma_N$ . The form functions  $\psi_i$  and  $\phi_j$  are given. Moreover,  $A$  is a coercive linear elliptic

operator of second order and  $\partial/\partial n_A$  denotes the co-normal derivative associated with  $A$ . Our main assumption is that  $g(x, y)$  and  $b(x, y)$  are non-decreasing *convex* functions in  $y$  for almost all  $x$ .

Generally speaking, Problem (COCP) can model applications in areas where the optimization of a static diffusion process is desired, subject to a given minimum state. For instance, we can model the static heating of a metallic workpiece by  $n$  heat sources; in this case, the set  $\mathcal{U} \subseteq \{0, 1\}^n$  models the switching of these sources,  $c_i$  is the cost of using source  $i$ ,  $A$  is the Laplace operator,  $g = 0$ , and  $b$  is of the form  $\sigma(|y|y^d - y_0^{d+1})$  with a constant  $y_0$ . The function  $y_{\min}$  is a point-wise minimal temperature that has to be reached in the metal piece.

By standard results, it follows that for each control vector  $u \in \mathbb{R}^n$  there exists a unique weak solution  $S(u)$  of the PDE in Problem (COCP). Our main result is the point-wise concavity of  $S$  under the given assumptions.

**Theorem 1.** *Under our assumptions, the mappings*

$$\text{conv}(\mathcal{U}) \ni u \mapsto S(u)(x) \in \mathbb{R} \quad \text{and} \quad \text{conv}(\mathcal{U}) \ni u \mapsto (\tau S(u))(x) \in \mathbb{R}$$

*are concave for almost every  $x \in \Omega$  and almost every  $x \in \Gamma_N$ , respectively.*

Here,  $\tau$  denotes the trace operator. The proof is similar to the proof of the weak maximum principle and uses deep results by Stampacchia; see, e.g., [2].

Based on Theorem 1, we can develop an outer approximation algorithm [1] for solving Problem (COCP). Linear cutting planes are produced using point-wise tangents of  $S(u)$ :

**Theorem 2.** *The operator  $S$  is Fréchet-differentiable. For all  $u^* \in \text{conv}(\mathcal{U})$  and almost all  $x \in \Omega$ , the inequality*

$$S(u^*)(x) + S'(u^*)(u - u^*)(x) \geq y_{\min}(x)$$

*is valid for all feasible solutions of (COCP).*

The resulting outer approximation algorithm is given as follows:

- (1) Set  $\mathcal{U}_0 := \mathcal{U}$ .
- (2) Minimize  $c^\top u$  over  $u \in \mathcal{U}_0$ , let  $u^*$  be the resulting optimizer.
- (3) Compute  $y^*$  solving

$$\begin{aligned} Ay + g(y) &= \sum_{i=1}^{\ell} u_i^* \psi_i && \text{in } \Omega \\ \frac{\partial y}{\partial n_A} + b(y) &= \sum_{j=\ell+1}^n u_j^* \phi_j && \text{on } \Gamma_N \\ y &= 0 && \text{on } \Gamma_D . \end{aligned}$$

- (4) If  $y^* \geq y_{\min}$  a.e., return  $u^*$  as optimal solution.
- (5) Choose some  $x^* \in \Omega$  with  $y^*(x^*) < y_{\min}(x^*)$  at random, add

$$y^*(x^*) + S'(u^*)(u - u^*)(x^*) \geq y_{\min}(x^*)$$

as linear inequality in  $u$  to  $\mathcal{U}_0$ , and go to Step 2.

It is now easy to show

**Theorem 3.** *If  $\mathcal{U}$  is bounded, the above algorithm terminates in finite time. With probability one, it returns a globally optimal solution to Problem (COCP).*

The main computational effort of the algorithm consists in solving an integer linear program (ILP) in Step (2), a nonlinear PDE in Step (3), and  $n$  linear PDEs in Step (3) in order to compute  $S'(u)$ . The solution of the nonlinear PDE can be improved by reoptimization techniques, taking into account the knowledge about  $S(u)$  acquired in earlier iterations.

We point out that a straightforward discretization of Problem (COCP) would result in a non-convex problem, by the presence of nonlinear equations. This means that the convexity of  $g$  and  $b$  would not be exploited at all, whereas our approach is based on this convexity. Experimental results show that our algorithm is capable of solving the combinatorial OCP of a semilinear Poisson equation with up to 200 binary controls to global optimality within a 5h time limit. Applied to the screened Poisson equation, problems with even 1800 binary controls are globally solvable. For a larger number of controls  $n$ , the running time is dominated by the time needed for solving the ILPs in Step (2) of the algorithm.

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### Strong Convex Nonlinear Relaxations of the Pooling Problem

CLAUDIA D'AMBROSIO

(joint work with J. Linderoth, J. Luedtke, J. Schweiger)

In this talk we focus on the standard pooling problem, i.e., a continuous, non-convex optimization problem arising in the petroleum industry and introduced by Haverly in 1978, see [1]. The problem consists of finding the optimal composition of final products obtained by blending in pools different percentages of raw materials. Formally, we are given a directed graph  $G = (V, A)$  where  $V$  is the set of vertices that is partitioned in three sets, i.e., the set of inputs or raw materials  $I$ , the set of pools or intermediate products  $L$ , and the set of outputs or final products  $J$ . Arcs  $(i, j) \in A$  link inputs to pools or outputs and pools to outputs. Each node and arc is subject to capacity constraints but the “complicating constraints” concern the requirements on the quality of certain attributes of the final products. The quality is a linear combination of the attributes of the raw materials and intermediate products that compose the final product. As the quality of the attributes of the intermediate products is not known in advance, the constraint shows bilinear terms.

Even if the problem is known since decades, only recently Alfaki and Haugland [2] proved that it is strongly NP-hard. The aim of this work is to strengthen the strongest known formulation, i.e., the so-called  $pq$ -formulation proposed by Tawarmalani and Sahinidis [3]. In particular, we studied a structured non-convex subset that is a relaxation of the original problem. We characterized its extreme points and derive the complete description of its convex hull under some assumptions. We prove that, for this case, the convex hull is characterized by nonlinear convex inequalities, i.e., it is non polyhedral. For the other cases we conjecture the full description of the convex hull. From the analysis of the structured non-convex subset we derive strong valid nonlinear convex inequalities for the standard pooling problem. Preliminary computational results on instances from the literature are reported and demonstrate the utility of the inequalities.

Future work and directions consist in (i) testing the inequalities on larger instances to confirm their effectiveness, (ii) proving the convex hull conjecture in the remaining considered cases, (iii) trying to identify a subset that better cast some of the characteristics of the pooling problem that were not considered.

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### Convex programming approaches for polynomial MINLP

ETIENNE DE KLERK

In this review talk, we consider the polynomial optimization problem:

$$(1) \quad f_{\min} := \min_{x \in \mathbb{R}^n} \{f(x) \mid g_j(x) \geq 0 \ (j \in \mathcal{J}), \ h_i(x) = 0 \ (i \in \mathcal{I})\},$$

where,  $\mathcal{I}$  and  $\mathcal{J}$  are index sets, and  $f$ ,  $g_j$  ( $j \in \mathcal{J}$ ), and  $h_i$  ( $i \in \mathcal{I}$ ) are all  $n$ -variate polynomials. We assume that the feasible set is compact, and use the notation  $[n] = \{1, \dots, n\}$  with power set  $2^{[n]} := \{I \mid I \subset [n]\}$ .

As a first step, we consider only binary variables, i.e. we set  $h_i(x) = x_i^2 - x_i$  ( $i \in \mathcal{I} = [n]$ ) in this case. Thus we consider the problem:

$$(2) \quad \min_{x \in \mathbb{R}^n} \{f(x) \mid g_j(x) \geq 0 \ (j \in \mathcal{J}), \ x \in \{0, 1\}^n\}.$$

Our goal is to reformulate this problem as an exponentially-sized semidefinite program, using the theory of combinatorial moment matrices.

We write an  $n$ -variate polynomial  $f$  of degree  $d$  as

$$f(x) = \sum_{\alpha \in \mathbb{N}_d^n} f_\alpha x^\alpha,$$

where  $x^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ , and  $\mathbb{N}_d^n = \{\alpha \in \mathbb{Z}^n \mid \alpha \geq 0, \sum_{i=1}^n \alpha_i \leq d\}$ . Since we deal only with binary variables for now, we may assume that  $\alpha \in \{0, 1\}^n$ .

We define the RLT linear (‘linearization’) operator from the  $n$ -variate polynomials of degree  $d$  to linear functionals on  $\mathbb{R}^{\binom{n+d-1}{d}}$ :

$$\sum_{\alpha \in \mathbb{N}_d^n} f_\alpha x^\alpha \mapsto \sum_{\alpha \in \mathbb{N}_d^n} f_\alpha y_\alpha,$$

i.e. we replace each monomial  $x^\alpha$  by new variable  $y_\alpha$ . Thus we may write  $y_I$  in stead of  $y_\alpha$  if  $I = \text{support}(\alpha) \subset [n]$ .

Note that under linearization:  $(\prod_{i \in I} x_i) \mapsto y_I$ .

**Definition 1.** Given a variable  $y \in \mathbb{R}^{2^{[n]}}$ , define the combinatorial moment matrix

$$M(y) = (y_{I \cup J})_{I, J \in 2^{[n]}}.$$

Note that, under linearization,  $(\prod_{i \in I} x_i) (\prod_{j \in J} x_j) \mapsto y_{I \cup J}$ .

Moreover, for any  $x \in \mathbb{R}^n$ , the matrix  $(\prod_{i \in I} x_i) (\prod_{j \in J} x_j)_{I, J \in 2^{[n]}}$  is positive semidefinite. It turns out that the condition  $M(y) \succeq 0$  (positive semidefinite) completely characterizes the convex hull of the vectors  $(\prod_{i \in I} x_i)_{I \in 2^{[n]}}$  with  $x \in \{0, 1\}^n$ , as the following theorem shows.

**Theorem 1** (Sherali-Adams [5], Lovász-Schrijver [4]).

$$\text{conv} \left\{ \left( \prod_{i \in I} x_i \right)_{I \in 2^{[n]}} \mid x \in \{0, 1\}^n \right\} = \left\{ y \in \mathbb{R}^{2^{[n]}} : y_\emptyset = 1, M(y) \succeq 0 \right\}.$$

In order to deal with the nonnegativity constraints, we also need the related concept of a *localizing matrix*.

Define, for  $j \in \mathcal{J}$ , the linear functional  $g_j * y$  via  $g_j(x) (\prod_{i \in I} x_i) \mapsto (g_j * y)_I$ , where the mapping is again the linearization operator.

**Definition 2.** Given a variable  $y \in \mathbb{R}^{2^{[n]}}$ , define the localizing matrix of  $g_j$  ( $j \in \mathcal{J}$ ) by

$$M(g_j * y) = ((g_j * y)_{I \cup J})_{I, J \in 2^{[n]}}.$$

Note that the localization matrix is the linearization of

$$g_j(x) \left[ \left( \prod_{i \in I} x_i \right) \left( \prod_{j \in J} x_j \right) \right]_{I, J \in 2^{[n]}} ,$$

and that the latter matrix is positive semidefinite for any feasible point of problem (2). Similarly to before, the conditions  $M(g_j * y) \succeq 0$  ( $j \in \mathcal{J}$ ) yield the required convex hull, in the sense of the next theorem.

**Theorem 2** (Laurent [3]). *The following two sets are the same:*

$$(i) \text{ conv} \left\{ \left( \prod_{i \in I} x_i \right)_{I \in 2^{[n]}} \mid x \in \{0, 1\}^n, g_j(x) \geq 0 (j \in \mathcal{J}) \right\}$$

$$(ii) \{y \in \mathbb{R}^{2^{[n]}} : y_\emptyset = 1, M(y) \succeq 0, M(g_j * y) \succeq 0 \ (j \in \mathcal{J})\}.$$

Based on this convex reformulation, one may define a hierarchy of convex approximations. The idea is to consider only principle submatrices of  $M(y)$  and  $M(g_j * y)$  indexed by subsets of cardinality at most  $t$ , where  $t$  is fixed. To this end, we define the *truncated moment matrix* by  $M_t(y)_{I,J} = y_{I \cup J}$  for  $I, J \in 2^{[n]}$ ,  $|I|, |J| \leq t$ .

**Definition 3** (Lasserre hierarchy of order  $t$  for  $2t \geq \text{deg}(f)$ ).

$$\ell(t) := \min_y \left\{ \sum_{|I| \leq 2t} f_I y_I \mid y_\emptyset = 1, M_t(y) \succeq 0, M_{t_j}(g_j * y) \succeq 0 \ (j \in \mathcal{J}) \right\},$$

where  $t_j = t - \lceil \text{deg}(g_j)/2 \rceil$ .

It follows from Theorem 2 that  $\ell(t)$  equals the optimal value of problem (2) for  $t \geq n$ . This was first shown in Lasserre [2].

We now return to the general polynomial optimization problem (1), and describe how the Lasserre hierarchy extends to the general problem. Since the exponents  $\alpha$  now no longer are 0-1 vectors in general, we have to define the moment and localizing matrices in a different way as follows.

- The moment matrix  $M(y)$  is defined via the linearization:  $x^\alpha x^\beta \mapsto y_{\alpha+\beta} =: M(y)_{\alpha,\beta}$ ;
- The localizing matrix  $M(g_j * y)$  is defined via:  $g_j(x) x^\alpha x^\beta \mapsto M(g_j * y)_{\alpha,\beta}$ .

If we only index by  $\alpha$  with  $|\alpha| := \sum_{i=1}^n \alpha_i \leq t$ , then we write  $M_t(y)$ , etc. This brings us to the general Lasserre hierarchy of approximations.

**Definition 4** (General Lasserre hierarchy of order  $t$  for  $2t \geq \text{deg}(f)$ ).

$$\ell(t) := \min_y \sum_{|\alpha| \leq 2t} f_\alpha y_\alpha$$

subject to

$$y_\emptyset = 1, M_t(y) \succeq 0, M_{t_j}(g_j * y) \succeq 0 \ (j \in \mathcal{J}), M_{s_i}(h_i * y) = 0 \ (i \in \mathcal{I}),$$

where  $t_j = t - \lceil \text{deg}(g_j)/2 \rceil$ ,  $s_i = t - \lceil \text{deg}(h_i)/2 \rceil$ .

Lasserre [1] showed that the values  $\ell(t)$  are well-defined and converge to the optimal value of problem (1), under an assumption that is a bit stronger than compactness of the feasible set.

**Theorem 3** (Lasserre [1]). *If we know a value  $R > 0$  such that a Euclidean ball of radius  $R$  contains the feasible set of problem (1), then  $\lim_{t \rightarrow \infty} \ell(t) = f_{\min}$ .*

In the talk we survey some known bounds on the convergence rate of  $f_{\min} - \ell(t)$  (seen as a sequence indexed by  $t$ ):

- For the combinatorial problem (2): the knapsack, maximum cut, minimum bisection, and maximum stable set problems;
- For the general problem (1): the special case where the feasible set is a simplex, the convex optimization case, as well as the general case.

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## An FPTAS for Concave Integer Quadratic Programming

ALBERTO DEL PIA

*Mixed-Integer Quadratic Programming* (MIQP) problems are optimization problems in which the objective function is quadratic, the constraints are linear inequalities, and some of the variables are required to be integers:

$$\begin{aligned}
 & \text{minimize} && x^\top Hx + h^\top x \\
 (1) \quad & \text{subject to} && Wx \leq w \\
 & && x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}.
 \end{aligned}$$

In this formulation,  $x$  is the  $n$ -vector of unknowns, while the remaining  $H$ ,  $h$ ,  $W$ ,  $w$  stand for the data in the problem instance:  $H$  is an  $n \times n$  symmetric matrix,  $h$  is an  $n$ -vector,  $W$  is an  $m \times n$  matrix, and  $w$  is an  $m$ -vector. MIQP problems arise in many areas, including economics, planning, and many kind of engineering design.

*Concave MIQP* is the special case of MIQP when the objective function is concave, which happens for example when the matrix  $H$  is negative semidefinite. Concave MIQP, like several other special cases of MIQP, is still an  $\mathcal{NP}$ -complete problem. This is even true in very restricted settings such as the problem to minimize  $\sum_{i=1}^n (w_i^\top x)^2$  over  $x \in \{0, 1\}^n$  [13], or when the concave quadratic objective has only one concave direction (one negative eigenvalue) [14]. Concave quadratic cost functions are often encountered in real-world integer programming models involving economies of scale (see [10], [15]), which corresponds to the economic phenomenon of “decreasing marginal cost”. *Concave QP* is the continuous version of concave MIQP, and is also  $\mathcal{NP}$ -complete [16], even when the concave quadratic objective has only one concave direction (one negative eigenvalue) [14]. Concave QP has been extensively studied. There are, however, few methods in the literature for concave MIQP. Branch-and-bound methods based on continuous relaxation and convex underestimating were proposed in [2], [3], [4], [5], [6].

If we assume that the number of integer and continuous variables  $n$  is fixed, then concave MIQP is polynomially solvable. Given a polyhedron  $P$ , Cook, Hartmann, Kannan, and McDiarmid [7] showed that in fixed dimension we can enumerate the

vertices of the integer hull  $\text{conv}\{x \in \mathbb{Z}^n : x \in P\}$  of  $P$  in polynomial time, and this result can be extended to the mixed-integer hull  $P_I = \text{conv}\{x \in \mathbb{Z}^p \times \mathbb{R}^{n-p} : x \in P\}$  by discretization [8, 11]. Since there is always an optimal point of concave MIQP that is a vertex of  $P_I$ , concave MIQP can now be solved in fixed dimension by evaluating all the vertices of  $P_I$  and by picking one with lowest objective value.

Since concave MIQP is  $\mathcal{NP}$ -hard, our focus is on approximation algorithms, which has been a very successful way to address  $\mathcal{NP}$ -hard optimization problems. In order to state our result, first it is necessary to give a definition of  $\epsilon$ -approximation: Consider an instance of MIQP, and let  $f(x)$  denote the objective function. We say that  $x^\diamond$  is an  $\epsilon$ -approximate solution if

$$|f(x^\diamond) - f_{\min}| \leq \epsilon |f_{\max} - f_{\min}|,$$

where  $f_{\min}$  and  $f_{\max}$  denote respectively the minimal and maximal value of the function on the feasible region. The concept of  $\epsilon$ -approximation that we adopt here has been used in earlier works, such as Nemirovsky and Yudin [12], Vavasis [18, 17], Bellare and Rogaway [1], de Klerk, Laurent, and Parrilo [9].

Our result, which is an extension to the mixed integer case of the celebrated result for concave QP by Vavasis [18], can then be stated as follows:

*Let  $k$  be the number of negative eigenvalues of  $H$ . There is an algorithm to find an  $\epsilon$ -approximate solution to concave MIQP. For fixed  $k$  and  $p$ , the running time of the proposed algorithm is polynomial in the size of the problem, and in  $1/\epsilon$ .*

Interestingly, the dependence on  $\epsilon$ ,  $k$  and  $p$  that we obtain might be expected. In fact, if we had a polynomial dependence on  $|\log \epsilon|$  for fixed  $k$ ,  $p$ , then we could solve Concave QP with  $k = 1$  in polynomial time [14], implying  $\mathcal{P} = \mathcal{NP}$ . Thus, assuming  $\mathcal{P} \neq \mathcal{NP}$ , polynomial dependence on  $1/\epsilon$  seems the best possible. Suppose now there exists an approximation algorithm whose running time is polynomial in  $1/\epsilon$  and in either  $k$  or  $p$ . Then we could solve 3SAT in polynomial time, implying once again  $\mathcal{P} = \mathcal{NP}$ .

The core structure of the algorithm combines and extends procedures used in MILP and in QP which have never been combined before. The key idea of the algorithm consists in iteratively subdividing the feasible region into two parts: one inner region where the mixed-integer points are “dense”, and an outer region where the mixed-integer points are “sparse”. The geometry of the mixed-integer points then allows us to employ tools used in the continuous QP setting in the inner region in order to obtain a good approximate solution. In the outer region, we use lattice algorithms from the MILP literature to subdivide the problem into a fixed number of lower-dimensional MIQPs.

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## A factorization heuristic for completely positive matrices

MIRJAM DÜR

(joint work with Patrick Groetzner)

The set  $\mathcal{CP}_n := \text{conv}\{xx^T \mid x \in \mathbb{R}_+^n\} = \{BB^T \mid B \in \mathbb{R}_+^{n \times k}\}$  is called the cone of completely positive matrices. Clearly,  $\mathcal{CP}_n$  is a subset of the positive semidefinite cone, and it is easy to see that it is indeed a proper subset. It is also not difficult to see that  $\mathcal{CP}_n$  is a closed, convex, pointed, and full dimensional cone, see also [2]

Completely positive matrices play an important role in quadratic and combinatorial optimization. De Klerk and Pasechnik [7] showed (cf. also [5]) that the stability number  $\alpha$  of a graph on  $n$  nodes with adjacency matrix  $A$  is given by

$$(1) \quad \alpha = \max\{\langle E, X \rangle \mid \langle A + I, X \rangle = 1, X \in \mathcal{CP}_n\},$$

where  $I$  denotes the identity matrix and  $E$  the all-ones matrix. This is remarkable, since it provides a formulation of the NP-hard stability number problem as a linear

optimization problem over a closed convex cone. Therefore, it is unsurprising that the membership problem of  $\mathcal{CP}_n$  is NP-hard, as shown in [9]. Interestingly, it is an open question whether checking  $A \in \mathcal{CP}_n$  is in the complexity class NP.

Later, Burer [6] showed that under mild conditions, the following two problems are equivalent:

$$\begin{array}{ll} \min & x^T Q x + 2c^T x \\ \text{s. t.} & a_i^T x = b_i \quad (i = 1, \dots, m) \\ & x \geq 0 \\ & x_j \in \{0, 1\} \quad (j \in B) \end{array} \quad \text{and} \quad \begin{array}{ll} \min & \langle Q, X \rangle + 2c^T x \\ \text{s. t.} & a_i^T x = b_i \quad (i = 1, \dots, m) \\ & a_i^T X a_i = b_i^2 \quad (i = 1, \dots, m) \\ & x_j = X_{jj} \quad (j \in B) \\ & \begin{pmatrix} 1 & x^T \\ x & X \end{pmatrix} \in \mathcal{CP}_{1+n}. \end{array}$$

This shows that any optimization problem with quadratic objective, linear constraints and (possibly) binary variables can be equivalently formulated as a linear problem over the cone of completely positive matrices.

Given a matrix  $A \in \mathcal{CP}_n$ , it is highly nontrivial to actually find a factorization  $A = BB^T$  with  $B \in \mathbb{R}_+^{n \times k}$ . Being able to compute a factorization would provide a certificate for  $A \in \mathcal{CP}_n$  and would hence be of interest for complexity reasons. Moreover, a factorization would help recover the solution of the underlying quadratic or combinatorial problem. As an example, consider the stability number problem (1). If an optimal solution  $X^*$  fulfills  $X^* = x^*(x^*)^T$ , then the support of  $x^*$  corresponds to a maximum stable set. On the other hand, if  $\text{rank}(X^*) > 1$ , then a factorization will yield more than one maximum stable set.

Approaches to develop factorization algorithms are [1, 3, 10, 11, 12]. However, these methods are either very difficult to implement, require a high computational effort, or work only for some matrices. In our talk, we propose a factorization heuristic which seems to work very quickly in many cases. However, for certain matrices (especially matrices of full rank on the boundary of  $\mathcal{CP}_n$ ) our heuristic fails.

Observe that for  $A \in \mathcal{CP}_n$ , the decomposition  $A = BB^T$  with  $B \in \mathbb{R}_+^{n \times k}$  is not unique. An example was given by Dickinson [8]:

$$\begin{pmatrix} 18 & 9 & 9 \\ 9 & 18 & 9 \\ 9 & 9 & 18 \end{pmatrix} = \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix} \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix}^T = \begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 0 & 3 & 0 \\ 3 & 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} 3 & 3 & 0 & 0 \\ 3 & 0 & 3 & 0 \\ 3 & 0 & 0 & 3 \end{pmatrix}^T.$$

Also note that the number of columns in  $B$  can vary. The minimal possible number of columns is called the cp-rank of  $A$ :

$$\text{cp}(A) = \inf\{k \in \mathbb{N} \mid \exists B \in \mathbb{R}_+^{n \times k}, B \geq 0, A = BB^T\}.$$

Determining the cp-rank of an arbitrary given matrix is also an open problem. However, upper bounds on  $\text{cp}(A)$  are given in [4]. Two factorizations  $A = BB^T = CC^T$  of the same size are related through the following well known result:

**Lemma 1.** *Let  $B, C \in \mathbb{R}_+^{n \times k}$ . Then  $BB^T = CC^T$  if and only if there exists an orthogonal matrix  $Q \in \mathbb{R}^{k \times k}$  with  $BQ = C$ .*

Our factorization heuristic is based on this lemma. Given an arbitrary factorization  $A = BB^T$ , the heuristic attempts to find an orthogonal matrix  $Q$  such that  $C := BQ \geq 0$ . This matrix  $C$  then provides the desired factorization  $A = CC^T$  of the completely positive matrix  $A$ .

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### Copositive programming and copositivity tests

GABRIELE EICHFELDER

(joint work with Carmo Brás, Joaquim Júdice)

A symmetric matrix  $A \in \mathcal{S}^n$  is called copositive if it generates a quadratic form which takes no negative values on the nonnegative orthant, i.e. in case it holds

$$x^\top Ax \geq 0 \quad \text{for all } x \in \mathbb{R}_+^n.$$

The problem of minimizing a linear form over the cone of copositive matrices  $\mathcal{COP}$  is called a copositive optimization problem. This type of optimization problem, and thus the task to evaluate whether a matrix is copositive, is of interest due to its relation to mixed-integer nonlinear optimization.

In a general setting this relation was given by Burer in [3]. He showed that a quadratic optimization problem with linear constraints has — under weak assumptions — a reformulation as (the dual of) a copositive optimization problem, also if some of the variables are binary. The considered quadratic optimization problems were of the form

$$\begin{aligned}
 \text{(QP)} \quad & \min x^\top Qx + 2c^\top x \\
 & \text{s.t. } Ax = b \\
 & \quad x_j \in \{0, 1\} \text{ for all } j \in B \\
 & \quad x \in \mathbb{R}_+^n
 \end{aligned}$$

with  $Q \in \mathcal{S}^n$ ,  $A \in \mathbb{R}^{m \times n}$ ,  $c \in \mathbb{R}^n$ ,  $b \in \mathbb{R}^m$ , and  $B \subseteq \{1, \dots, n\}$ . The mentioned reformulation was originally given as a linear optimization problem over the cone of completely positive matrices  $\mathcal{CP}$  defined by

$$\mathcal{CP} := \text{conv}\{xx^\top \mid x \in \mathbb{R}_+^n\}.$$

The new problem is then

$$\begin{aligned}
 \text{(CP)} \quad & \min \langle Q, X \rangle + 2c^\top x \\
 & \text{s.t. } Ax = b \\
 & \quad \text{Diag}(AXA^\top) = b \circ b \\
 & \quad x_j = X_{jj} \text{ for all } j \in B \\
 & \quad \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \in \mathcal{CP} \\
 & \quad x \in \mathbb{R}^n, X \in \mathcal{S}^n.
 \end{aligned}$$

Here,  $b \circ b := (b_1^2, \dots, b_m^2)^\top$  and the inner product in  $\mathcal{S}^n$  is defined by  $\langle A, B \rangle := \text{trace}(AB)$  for  $A, B \in \mathcal{S}^n$ , as usual.

Under the assumption that the equality constraints  $Ax = b$  imply for any  $x \in \mathbb{R}_+^n$  that  $x_j \in [0, 1]$  for all  $j \in B$ , the problem (QP) is equivalent to the problem (CP). Moreover, it holds that

$$\mathcal{CP} = \mathcal{COP}^* \quad \text{and} \quad \mathcal{CP}^* = \mathcal{COP}.$$

Thus, the dual problem of (CP) is a copositive optimization problem.

The difficulty of a copositive optimization problem lies in the difficulty of checking whether it holds  $A \in \mathcal{COP}$  for a given matrix  $A \in \mathcal{S}^n$ . Checking this membership to the copositive cone is an co-NP-complete problem, cf. [5, 6]. Various authors have proposed copositivity tests in the literature, but there are only a few implemented numerical algorithms which apply to general symmetric matrices without any structural assumptions or dimensional restrictions and which are not just recursive, i.e., do not rely on information taken from all principal submatrices.

In this talk, next to presenting the above relations to MINLPs, I shortly recall two copositivity tests of the last years (originally given by Bundfuss and Dür in [4] and by Bomze and Eichfelder in [1]). Both algorithms make use of the fact that

$$A \in \mathcal{COP} \Leftrightarrow \min\{x^\top Ax \mid e^\top x = 1, x \in \mathbb{R}_+^n\} \geq 0$$

(with  $e \in \mathbb{R}^n$  the all-one vector) and are based on a branch and bound algorithm. However, they use different branching and bounding criteria.

In the remaining of the talk I present some more recent copositivity tests as given in [2]. These new tests make use of necessary and sufficient conditions which require the solution of linear complementarity problems (LCPs). Methodologies involving Lemke's method, an enumerative algorithm and a linear mixed-integer programming formulation are proposed to solve the required LCPs. Numerical results which compare the new tests with the copositivity tests from [1, 4, 7] are presented.

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### Aspects of Time in Mixed-Integer (Non-) Linear Optimization

ARMIN FÜGENSCHUH

George Dantzig [6] reported that his linear programming algorithm was criticized right after his inaugural presentation in 1948 [4] for not being able to deal with nonlinear problems that are ubiquitous in real-world applications. However, by using linear inequalities and piecewise linear approximations, most nonlinear functions that are encountered in such applications can be sufficiently approximated. Over the past six decades, several researchers published model formulations to model a piecewise linear function (that approximates a given nonlinear function) in one or several dimensions, for example [22, 5, 2, 1, 28, 24, 21, 23, 29, 30]. These formulations differ in the way they use binary variables and the number of binary variables. All these approaches have in common that the piecewise-linear function has to be defined before the model is formulated, and does not change during the MILP solution process. A more modern approach that avoids this disadvantage was described by Smith and Pantelides [25] and Tawarmalani and Sahinides [27]. Here the approximation of the nonlinear function is created during the branch-and-cut solution process by adding further cutting planes and carrying out spatial branching. A direct comparison on a nonlinear network flow model indicates that this method is actually much faster [13]. For certain types of nonlinear functions, such as second order cone constraints of the form  $\sqrt{x_1^2 + \dots + x_n^2} \leq t$ , there exist

very accurate linear approximations that embed this cone in a higher dimensional space by introducing auxiliary variables [3, 19]. These reformulations can be used to solve practical nonlinear mixed-integer problems with MILP solvers, such as soft rectangle packing problems [17], or car routing problems in railway freight transportation [16].

Despite the initial critics about the “limited scope” of linear programming (LP), it turned out to become a huge success, and is considered as one of the most important mathematical discoveries (or inventions) of the 20th century. LP is the working horse for solving (mixed-) integer and thus many combinatorial optimization problems, starting from the traveling salesman problem by Dantzig, Fulkerson, and Johnson in 1954 [7]. Soon after, more complex logistic and transportation problems were addressed, such as the truck-use problem by Dantzig and Ramser in 1959 [8]. The transport of goods often requires time synchronization of different work steps. Shipments can be picked up or delivered only in certain time windows, a handover of goods between two players can only take place when both are at the same time in the same place. A useful optimization model for such applications must consider this aspect. While this is evident from a practical side, the integration of the time aspect in MILP models leads to algorithmically difficult problems. Most frequently encountered in the literature is one of the following two ways to include the time aspect in an optimization model.

In the continuous time modeling, time is described by real-valued variables, indicating the time relative to a specified start time in a defined unit (e.g., seconds). For each incident  $i$  (for example, an object being at a certain location, or a machine working on a certain job), a continuous time variable  $t_i$  describes when this incident is going to happen. For example, in bus or train scheduling application [11, 15], a tour of length  $d_i$  is started at time  $t_i$ . If tours  $i$  and  $j$  are connected (i.e., served by the same bus or train directly after another), then  $t_j - (t_i + d_i) \geq 0$ . The connection is modeled by the binary variable  $x_{i,j}$ . Hence the precedence relation is formulated by the nonlinear constraint  $(t_j - (t_i + d_i))x_{i,j} \geq 0$ . In order to apply mixed-integer linear solvers, one has to linearize this constraint. To this end, in the (in-) famous “big- $M$ -method”, a parameter  $M$  is introduced, which allows to linearize the constraint to  $t_j - (t_i + d_i) \geq M(x_{i,j} - 1)$ . Although one achieves a mixed-integer linear formulation, it usually has a weak LP-relaxation, which leads to less pruned nodes, thus large branch-and-bound trees, and thus large solution times.

An alternative to the big- $M$  continuous time formulation is provided by a discrete modeling of time. The available finite time horizon is sliced into intervals of fixed unit length (e.g., 5 minutes). Then for each incident  $i$  and each time step  $t$  a binary variable  $x_{i,t}$  is introduced, which indicates, if incident  $i$  happens in time step  $t$ . In this purely discrete setting, often better LP relaxations are achieved. However, there is a trade-off between accuracy and solution time: If the time is sliced into too many pieces, then the resulting models are of enormous size, which are impractical for a numerical solution process. When carefully used, small to

medium size real-world optimization problems can be solved in reasonably short time [26].

A new way of dealing with time called “time-free relaxation” was introduced in [18]. Here the time index of all variables  $x_{i,t}$  is projected away, so that variables  $x_i$  remain. Then all constraints have to be adapted accordingly. This results in very small, but still mixed-integer models, that usually can be solved very easily. In general, they do not yield feasible solutions to the original problem “with time”, and it is in fact a difficult problem to decide if a projected solution has a feasible counterpart with proper times attached to it. When embedded in a branch-and-bound search, where a time-free master problem interacts with time-indexed subproblems to solve this inverse problem, the overall solution process can be faster, compared to a solution over the full time-indexed problem. A refinement of this method is a promising direction of further research.

The individual challenges imposed by mixed-integer optimization over time and mixed-integer optimization with nonlinear constraints are coupled when they are blended with differential equation constraints (ODEs or PDEs). These constraints usually arise in the description of technical systems to model physical properties. Even a simple PDE, such as the transport equation, leads to numerically difficult optimization problems when handed over to a standard MILP solver [20, 12]. One way to include PDEs into a MIP is by a finite difference discretization in time and space of the PDE. Even moderate discretization step sizes lead to instances with a huge number of variables and constraints. Although one can obtain a linear model (for the transport PDE, for instance), the solver tend to have numerical problems on these instances, so certain steps of the classical MILP solution process have to be revisited, for example, the bounds strengthening routines in the presolve phase [9]. Amazingly, putting one of the most simple problems from the area of combinatorial optimization, namely the shortest path problem, together with one of the most simple PDE, namely the heat equation, leads due to their combination to a new and challenging problem, which we call the coolest path problem [10].

ODEs and PDEs describe the physics to a very high degree of accuracy. However, in order to obtain the “right” combinatorial decisions, it can be beneficial not to work with the full complexity of the DE, but with some simpler approximation. To start with, a hierarchy of models must be derived, from fine to coarse, and afterwards the right level to formulate the mixed-integer optimization problem can be chosen among that hierarchy. In [14] this approach was demonstrated using traffic flows in networks.

Clearly, mixed-integer nonlinear dynamic optimization with differential equation constraints is full of challenging problems and has many practical applications, so that it is worth to devote more research on this emerging problem class.

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## Unifying randomization techniques and semidefinite and set-copositive relaxations of binary problems

FLORIAN JARRE

(joint work with Felix Lieder, Fatemeh Bani Asadi Rad)

One of the most successful techniques for approximating a local solution of an NLP is the SQP-approach solving a linearly constrained quadratic program at each iteration. The crucial point of the SQP approach is defining the objective function of the SQP subproblem by the Hessian of the Lagrangian (rather than by the Hessian of the objective function). A suggestion is discussed as how to maintain this crucial point for MINLP, i.e. in the presence of binary and integer constraints. The resulting subproblems take a form closely related to the one considered in Burer [6]. Burer proposed an exact relaxation of a QP with mixed binary constraints as a program over the completely positive cone. This relaxation is computationally not tractable, and several authors have considered weaker relaxations replacing the completely positive cone with the doubly nonnegative cone or with the semidefinite cone.

Several aspects of such reformulations are discussed, aspects that may be crucial for an iterative approach such as SQP, in particular, results relating to

- (1) the tightness and the key condition,
- (2) the computational cost,
- (3) and the generation of feasible solutions from the relaxation.

The heuristics of Goemans and Williamson [7] has proved to be a valuable practical and theoretical tool for approximating the solution of max-cut problems. The key of its numerical success is a combination of the availability of efficient algorithms exploiting the particular structure of the semidefinite relaxation, see e.g. [9], and a provable bound for the average behavior of the heuristics as well as the availability of local refinement strategies. The result [7] was soon set into perspective [10] but it remains an important practical tool that has been implemented with a branch and cut algorithm [12] in a slightly extended framework

of binary quadratic programs for which the assumptions of [7] do not necessarily hold, and for which the theoretical bound is thus no longer available, but which nevertheless yields excellent numerical approximations of the optimal solution.

The result by Goemans and Williamson refers to a  $\{-1, 1\}$ -formulation while the completely positive reformulation is based on a  $\{0, 1\}$ -formulation making the combination of both results a bit technical. It is clear that, in principle, both formulations must be equivalent. Following the presentation in [8, 11], it is shown that the Goemans-Williamson randomization technique can be generalized for quadratically constrained binary programs in either formulation and that these binary programs – under some additional assumption – can also be rewritten as duals of set-copositive linear optimization problems. The set-copositive cone in this reformulation only depends on the dimension and is independent of the problem data.

Earlier works combining instances of both formulations are, for example, the work by Bertsimas and Ye [3] and Benson and Ye [2] who modified the approach by Goemans and Williamson to the max-clique problem. Here, the approach of [3, 2] is adapted in a way so that the simple structure of the semidefinite max-cut relaxation is fully maintained except from one additional linear equality constraint that can be handled by means of rank-one-updates. The resulting relaxation is somewhat weaker than the Lovasz number in [3, 2] but much faster computable, in particular for larger graphs with moderate edge density. In addition, it turns out that also for the relaxation by Burer, all the linear constraints can be accumulated into two linear constraints without changing the optimal solution of the relaxation. This transformation is applicable to semidefinite, doubly nonnegative, and completely positive programs.

Finally, a set-completely-positive reformulation, see [1], is presented that does not require a key condition. The set-completely-positive cone is independent of the problem data and some of the heuristics for optimizing over the completely positive cone can be transferred in a straightforward fashion to such set-completely-positive cones. A possible generalization to the format of SQP subproblems and an implementation for MINLP are the subject of future research.

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## Optimal Control Problems with Discrete Variables: Applications, Methods, and Constraints

MATTHIAS GERDTS

The talk provides an overview on theoretical properties of and numerical approaches for optimal control problems with ordinary differential equations and differential-algebraic equations (DAEs) with discrete-valued controls. Such problems appear in various applications in engineering and economics, where discrete controls are used to model decisions, switches, or hybrid systems. A typical example is the optimization of gear shifts in a car or a truck, compare [2].

We investigate DAE optimal control problems of the following type:

*Minimize*  $\varphi(x(0), x(1))$  *w.r.t.*  $x \in W^{1,\infty}([0, 1], \mathbb{R}^{n_x})$ ,  $y \in L^\infty([0, 1], \mathbb{R}^{n_y})$ ,  $u \in L^\infty([0, 1], \mathbb{R}^{n_u})$  *subject to the constraints*

$$\begin{aligned} x'(t) &= f(x(t), y(t), u(t)), \\ 0 &= g(x(t)), \\ u(t) &\in \mathcal{U}, \\ 0 &= \psi(x(0), x(1)). \end{aligned}$$

Herein,  $(x, y)$  denotes the differential state,  $u$  the control,  $\mathcal{U} \subset \mathbb{R}^{n_u}$  the control set (can be a discrete set), and  $\varphi, f, g, \psi$  are sufficiently smooth functions. Exploitation of a proof technique in [1], which uses a variable time transformation to transform the discrete optimal control problem into an equivalent optimal control problem without discrete-valued controls but with mixed control-state constraints, allows to prove necessary conditions in terms of a global minimum principle. Under appropriate assumptions on the index of the DAE there exist nontrivial multipliers  $\ell_0 \geq 0$ ,  $(\ell_0, \zeta, \sigma, \lambda_f, \lambda_g) \neq 0$  such that the following conditions hold at a strong

local minimum  $(x_*, y_*, u_*)$  of the DAE optimal control problem:

$$\begin{aligned}\lambda_f' &= -\nabla_x H(x_*(t), y_*(t), u_*(t), \lambda_f(t), \lambda_g(t)), \\ 0 &= \nabla_y H(x_*(t), y_*(t), u_*(t), \lambda_f(t), \lambda_g(t)), \\ \lambda_f(0)^\top &= -(\ell_0 \varphi'_{x_0}(x_*(0), x_*(1)) + \sigma^\top \psi'_{x_0}(x_*(0), x_*(1)) + \zeta^\top g'_x(x_*(0))), \\ \lambda_f(1)^\top &= (\ell_0 \varphi'_{x_f}(x_*(0), x_*(1)) + \sigma^\top \psi'_{x_f}(x_*(0), x_*(1))), \\ (u_*(t), y_*(t)) &\in \operatorname{argmin}_{(u,y) \in M(x_*(t))} H(x_*(t), y, u, \lambda_f(t), \lambda_g(t))\end{aligned}$$

where

$$H(x, y, u, \lambda_f, \lambda_g) = \lambda_f^\top f(x, y, u) + \lambda_g^\top g'_x(x) f(x, y, u)$$

denotes the Hamilton function and  $M(x) := \{(u, y) \mid g'_x(x) f(x, y, u) = 0\}$ . Moreover, the Hamilton function is constant at the optimal solution. Details of the proof can be found in [4, Chapter 7] for index-2 DAEs and in [5] for index-1 DAEs.

The proof technique gives also rise to a numerical method, which exploits the variable time transformation, compare [11, 3]. The numerical performance is demonstrated for an example from virtual testdrives. An alternative approach uses a relaxation of the discrete optimal control problem in combination with an a posteriori rounding strategy, compare [10, 9]. Extensions of the latter sum-up-rounding strategy towards model-predictive control can be found in [6].

Particular difficulties arise, if switching costs or constraints depending on the discrete-valued control have to be considered. The latter can be reformulated using so-called vanishing constraints and tailored optimization methods have to be derived, compare [7]. An example from aircraft trajectory optimization with control dependent velocity constraints, see [8], concludes the talk.

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## **Relaxations for Convex Nonlinear Generalized Disjunctive Programs, their Application to Nonconvex Problems and to Logic-based Outer Approximation Algorithm**

IGNACIO E. GROSSMANN

This talk deals with the theory of reformulations and numerical solution of generalized disjunctive programming (GDP) problems, which are expressed in terms of Boolean and continuous variables, and involve algebraic constraints, disjunctions and propositional logic statements. We propose a framework to generate alternative MINLP formulations for convex nonlinear GDPs that lead to stronger relaxations by generalizing the seminal work by Egon Balas [1] for linear disjunctive programs. We define for the case of convex nonlinear GDPs an operation equivalent to a basic step for linear disjunctive programs that takes a disjunctive set to another one with fewer conjuncts. We show that the strength of relaxations increases as the number of conjuncts decreases, leading to a hierarchy of relaxations. We prove that the tightest of these relaxations allows in theory the solution of the convex GDP problem as an NLP problem. We present a guide for the generation of strong relaxations without incurring in an exponential increase of the size of the reformulated MINLP. We apply the proposed theory for generating strong relaxations to a dozen convex GDPs which are solved with an NLP-based branch and bound method. Compared to the reformulation based on the hull relaxation, the computational results show that with the proposed reformulations significant improvements can be obtained in the predicted lower bounds, which in turn translates into a smaller number of nodes for the branch and bound enumeration. We then briefly describe an algorithmic implementation to automatically convert a convex GDP into an MILP or MINLP using the concept of basic steps, and applying both big-M and hull relaxation formulations to the set of disjunctions.

We address the extension of the above ideas to the solution of nonconvex GDPs that involve bilinear, concave and linear fractional terms. In order to solve these nonconvex problems with a spatial branch and bound method, a convex GDP relaxation is obtained by using suitable under- and over-estimating functions of the nonconvex constraints. In order to predict tighter lower bounds to the global optimum we exploit the hierarchy of relaxations for convex GDP problems. We

illustrate the application of these ideas in the optimization of several process systems to demonstrate the computational savings that can be achieved with the tighter lower bounds. We also discuss recent work aimed at automating convex GDP reformulations into MILP/MINLP models in which basic steps are applied selectively and a hybrid of big-M and hull reformulation constraints is used. In order to decrease the size of these reformulations, an algorithm is presented for the derivation of cutting planes derived from basic steps and that are used to strengthen big-M models. Computational experience is reported on a set over 30 instances of varying sizes and complexity.

We also present an alternative logic-based outer-approximation algorithm to find the global solution of non-convex GDPs. The general idea of the algorithm is to have a master MILP that overestimates the feasible region of the GDP. This master problem provides a valid lower bound (in a minimization problem), and the selection of only one disjunctive term in each of the disjunctions. With this alternative provided by the master problem, an NLP subproblem is solved to global optimality. This NLP subproblem is smaller and simpler than the continuous relaxation of the MINLP reformulation of the original GDP. After solving this subproblem, infeasibility or optimality integer cuts can be added to the master problem. This basic algorithm has the advantage of solving only small NLP problems to global optimality, instead of solving a larger MINLP to global optimality from the beginning. Furthermore, by using GDP as framework the NLP subproblem is smaller and simpler than an equivalent method directly applied to the MINLP reformulation. Even with these advantages, the convergence of the algorithm is slow and it may have difficulties finding good or optimal solutions. In order to improve the performance of this logic-based outer approximation, we implement three main features: derivation of additional cuts, partition of the algorithm in two stages, and parallelization of the algorithm.

In the first improvement we develop a novel method to derive a cutting plane in each of the disjunctive terms selected by the master problem. We obtain this cut by solving to global optimality one NLP for each of the selected disjunctive terms. This NLP minimizes the distance between the solution found by the master problem, and a point that lies in the tightest possible convex region that contains the nonconvex region described by the disjunctive term. The idea of solving this NLP to obtain a cut is similar to the well-known concept of the separation problem in MILP and convex MINLP. A second improvement in the algorithm is its partition into two phases. The first phase seeks to find a good feasible solution, while the second phase provides a rigorous lower bound. The first phase tests many alternatives and evaluates the NLP subproblems only for a few seconds. If an NLP subproblem provides a feasible solution, it is a valid upper bound. If the NLP is proven infeasible within that time period, then a feasibility cut is derived, and it is valid for the original MINLP. If the NLP does not find a feasible solution within the given time, an infeasibility cut is derived and used for the first phase. However, this cut is not valid for the original MINLP, so it is discarded in the second phase. Note that the first phase provides valid upper bounds when found,

but it does not provide a valid lower bound in general. For the second phase, the invalid cuts found in phase 1 are removed. After this, the rigorous algorithm previously described is solved (without stopping the NLP subproblems until they are solved to global optimality or proven infeasible). In this second phase a stronger MILP relaxation is used to provide good lower bounds. The third improvement in the algorithm is to parallelize the derivation of cutting planes and solution of subproblems. This parallelization is performed by obtaining a pool of solutions from the master problem. The cut derivation and subproblem solution is then performed in parallel for each of the solutions in the pool.

We illustrate the application of this algorithm with several GDP process networks examples. In some cases, process networks are difficult to solve as MINLPs, but easy NLPs to solve for a given fixed structure. This characteristic makes the logic based outer-approximation an attractive method for solving these type of problems. We compare the solution of these problems using the described algorithm against global optimization solvers. The results show that the algorithm generally finds better solutions faster, and with a smaller optimality gap.

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## Approximation properties of complementarity problems from mixed-integer optimal control

CHRISTIAN KIRCHES

(joint work with Michael N. Jung, Felix Lenders, Sebastian Sager)

We extend recent work [5, 6, 8] on the numerical solution of mixed-integer nonlinear optimal control problems (MIOCPs) to the case of discrete control functions subject to combinatorial constraints. In more detail, we are interested in computing optimal state and control trajectories  $(x^*, u^*, v^*)$  that solve the problem

$$(\text{MIOCP}) \quad \left\{ \begin{array}{ll} \min_{x,u,v} & \int_0^T L(x(t), u(t), v(t)) dt + E(x(T)) \\ \text{s.t.} & \dot{x}(t) = f(x(t), u(t), v(t)) \quad \text{a.e. } t \in [0, T] \\ & 0 \leq c(x(t), u(t), v(t)) \quad \text{a.e. } t \in [0, T] \\ & 0 \leq d(x(t), u(t)) \quad \text{a.e. } t \in [0, T] \\ & 0 \left\{ \begin{array}{l} \leq \\ = \end{array} \right\} r(\{x(t_i)\}) \quad \{t_i\} \subset [0, T] \\ & v(t) \in \Omega := \{v^1, \dots, v^{n_\Omega}\} \subset \mathbb{R}^{n_v} \quad \text{a.e. } t \in [0, T]. \end{array} \right.$$

Prominent examples of such systems include problems with restrictions on the number of switches permitted, or problems that minimize switch cost. We present a computational approach to MIOC that is based on partial outer convexification of (MIOCP) with respect to the discrete control  $v(t)$ , cf. [5], and on a vanishing constraint formulation for the combinatorial constraint  $0 \leq c(x(t), u(t), v(t))$  on the integer control, cf. [1, 2]. This setting has been shown to be a powerful approach for solving practically relevant problems, e.g. [4]. We extend a theorem due to [6] to this setting and prove that, after relaxation, the integrality gap is zero in appropriately chosen function spaces. After discretization of (MIOCP) in time, the integrality gap can be made arbitrarily small by selecting a sufficiently fine grid. In order to construct an integer feasible solution from the relaxed optimal one, a MILP can be solved [7] or a rounding scheme can be applied. We extend a sum-up rounding (SUR) scheme due to [8] to the case of combinatorial constraints. Our scheme permits to constructively obtain an  $\varepsilon$ -feasible and  $\varepsilon$ -optimal discrete control. We derive two tighter upper bounds on the integer control approximation error made by SUR. For unconstrained discrete controls, we reduce the approximation error bound from  $\mathcal{O}(n_\Omega)$  to  $\mathcal{O}(\log n_\Omega)$  asymptotically. We further show that this new bound is tight. For constrained discrete controls, we prove that an approximation error bound of  $\mathcal{O}(n_\Omega)$  holds and is tight. The presented results can be found in [3], and applications to MIOCPs from practical and real-world applications can be found in, e.g., [2, 4, 5].

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## Comparing polyhedral relaxations via volume

JON LEE

With W. Morris in 1992, I introduced the idea of comparing polytopes relevant to combinatorial optimization via calculation of  $n$ -dimensional volumes. That work involved deriving exact formulae for volumes in well-structured situations, followed by relevant asymptotic analysis. The motivation was MINLP. I will review some of that work related to fixed-charge problems, to give a flavor of the type of results. Some years later, in 2007, I made some computations on separable convex-quadratic objectives which correlated with our theoretical results. The message is that there are clear situations where a simpler relaxation may be only slightly weaker, and so it may be preferred in the context of global optimization.

In 2015, I obtained results with E. Speakman, relevant to the spatial branch-and-bound approach to global optimization. In this new work, we calculate exact expressions for 4-dimensional volumes of natural parametric families of polytopes relevant to different convex relaxations of trilinear monomials. As a consequence, we have practical guidance: (i) for tuning an aspect of spatial branch-and-bound implementations [1], (ii) at the modeling level. This work is clearly just a sample of what can be done to more deeply analyze the low-dimensional functions that are in modeling trickery and spatial branch-and-bound libraries.

Other related work is [5] and [6]. A nice open problem is:

For  $n \geq 2$ , the *Boolean Quadric Polytope*  $\mathcal{P}_n$  is the convex hull in dimension  $d = n(n + 1)/2$  of the 0/1 solutions to  $x_i x_j = y_{ij}$  for all  $i < j$  in  $N := \{1, 2, \dots, n\}$ . Give a formula or good bounds for the  $d$ -dimensional volume of  $\mathcal{P}_n$ .

**Comments:** The polytope  $\mathcal{P}_n$  is contained in  $\mathcal{Q}_n$ , the solution set of the linear inequalities:  $y_{ij} \leq x_i$ ,  $y_{ij} \leq x_j$ ,  $x_i + x_j \leq 1 + y_{ij}$ , for all  $i < j$  in  $N$ . In [5], we demonstrated that the  $d$ -dimensional volume of  $\mathcal{Q}_n$  is  $2^{2n-d} n! / (2n)!$ . So this is an upper bound on the  $d$ -dimensional volume of  $\mathcal{P}_n$ . We would like to see a significant improvement in this upper bound and/or a non-trivial lower bound. There is quite

a lot known about further linear inequalities satisfied by  $\mathcal{P}_n$ , so there are avenues to explore for trying to get a significant improvement in the upper bound.

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### Mixed-Integer PDE-Constrained Optimization

SVEN LEYFFER

(joint work with Pelin Cay, Drew Kouri, and Bart van Bloemen Waanders)

Many complex scientific and engineering applications can be formulated as optimization problems constrained by partial differential equations (PDEs) with both continuous and integer decision variables. This new class of mathematical problems, called mixed-integer PDE-constrained optimization (MIPDECO) [4], must overcome the combinatorial challenge of integer decision variables combined with the numerical and computational complexity of PDE-constrained optimization.

Examples of MIPDECO include the remediation of contaminated sites and the maximization of oil recovery, which involve flow through porous media and the optimization of wellbore locations and optimal flow rates [2], and operational schedules [1]. Related applications also arise in the optimal scheduling of shale-gas recovery [6]. Next-generation solar cells face complicated geometric and discrete design decisions to achieve perfect electromagnetic performance [5]. In disaster-recovery scenarios, such as oil spills [7], and hurricanes [3], resources must be scheduled to mitigate the disaster while adjusting to the underlying dynamics for accurate forecasts. Other science and engineering examples include the design, control, and operation of wind farms and gas networks.

Each of these applications combine discrete decision variables with complex multiphysics simulation. Until recently, these grand challenge problems have been

regarded as computationally intractable. Formally, we state a mixed-integer PDE-constrained optimization problem as

$$\begin{aligned}
 (1) \quad & \underset{u,w}{\text{minimize}} && \mathcal{F}(u, w) \\
 & \text{subject to} && \mathcal{C}(u, w) = 0, \\
 & && \mathcal{G}(u, w) \leq 0, \\
 & && u \in \mathcal{D}, \text{ and } w \in \mathbb{Z}^p \text{ (integers)},
 \end{aligned}$$

which is defined over a domain  $\Omega$ . We use  $x, y, z$  to indicate spatial coordinates of the domain  $\Omega$  and  $t$  to denote time. The objective function of (1) is  $\mathcal{F}$ ,  $\mathcal{C}$  are the equality constraints, and  $\mathcal{G}$  are inequality constraints. The equality constraints include the PDEs as well as boundary and initial conditions. We denote the continuous decision variables of the problem by  $u(t, x, y, z)$ , which includes the PDE states, controls, or design parameters. We denote the integer variables by  $w(t, x, y, z)$ , which may include design parameters that are independent of  $(t, x, y, z)$ . Thus, in general, problem (1) is an infinite-dimensional optimization problem, because the unknowns,  $(u, w)$ , are functions defined over the domain  $\Omega$ , although we avoid a formal discussion of function spaces in this paper.

We review existing approaches for solving these problems, and we highlight their computational and mathematical challenges. We introduce a benchmark set for this class of problems and present some early numerical experience using both mixed-integer nonlinear solvers and nonlinear rounding heuristics.

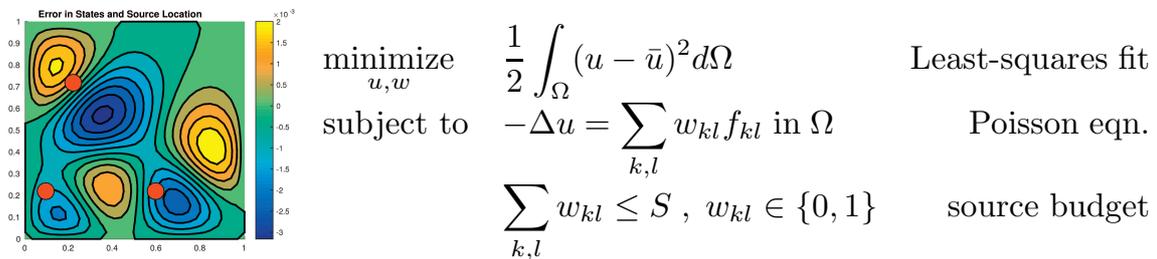


FIGURE 1. Formulation and solution of a simple source inversion model.

One example of our benchmark problems is a simple source inversion problem based on Laplace’s equation with Dirichlet boundary conditions, which is motivated by groundwater flow applications. The goal is to match observations,  $\bar{u} \in \Omega$  by selecting possible sources from a set of possible sources using binary variables. We prefer the use of binary variables, because an alternative formulation, which models the source location as continuous variables, results nonlinear (i.e. nonconvex) constraints. We discretize the PDE with a five-point finite difference stencil using an equidistant meshsize of  $h = 1/32$ , and we limit the number of sources to  $S = 3$ . The resulting discretized problem is a convex mixed-integer quadratic program. We solve the discretized problem using MINOTAUR’s branch-and-bound solver, which searches 759 nodes in 69s of CPU time on an Intel i7 core. Figure 1 shows the optimal selection of sources as red dots and the deviation from  $\bar{u}$ , as well as the problem formulation.

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## Big Data & Mixed-Integer Non Linear Programming

ANDREA LODI

(joint work with Marie-Claude Côté)

In this talk we discuss some personal viewpoints in the domain of so-called *Big Data* that open interesting lines of research for Mathematical Optimization [4] and, more specifically, Mixed-Integer Non Linear Programming [1] (MINLP). We do that by using two simple and informative examples of non-necessarily-big data.

- (1) The first example concerns a face recognition system put in place in a mall somewhere in the US. Main purpose of the system was security. After collecting data for some time, it has been observed that the large majority of the clients entering in the mall around lunch time (11AM - 3PM) was composed by Asian-American people. The company owning the mall implemented two simple actions: (i) revised the shifts of the employees so as that (most of) the Asian-American ones were on duty in that time window and (ii) hired new Asian-American employees. The overall effect has been a huge increase in sales.
- (2) The second example is in the retail industry and concerns a promotion execution in an integrated real-time decision support system. Based on the forecast, 300 blouses are sent for the promotion that starts at 5PM

on Friday. By 10PM 180 blouses have sold and an intra-day pace-based forecasting engine detects a potential stock out situation and generates an alert: at this pace blouses will be sold out by 2PM on Saturday. Retailer has a relatively nimble supply chain. The system generates an order at the DC to be put on the regular 9AM shipment. Shelves are full and customers are happy. Revenues are robust and promotional efficiency is high. But the weather forecast for Saturday is terrible, and the likely surge in sales on Friday is a reflection of that. In addition, shoppers have been “tweeting” about this deal and that has generated a buzz and anticipated traffic and sales. Real-time demand-sensing allows retailers to improve the execution of their promotions and to optimize future promotional plans.

Example (1) shows that automatic collection of data can lead to the definition of new (optimization) problems. Disseminating sensors (including mobile devices) everywhere has become cheap (and cool!) but the real challenge is taking decisions over the collected (complex) data. It is not completely clear if the (applied) optimization problems we were used to solve in contexts as diverse as routing, supply chain and logistics, telecommunication, etc. are still there or, instead, have radically changed.

The spirit of such a change is shown by example (2): the end-users “behavior” is putting more and more pressure on the decision makers and, by transitivity, on the optimizers. This is not true only in the retail industry but virtually in any other in which a service is delivered:

- routing, I can check with my mobile device where cabs/buses are located;
- traffic management, I am aware of congestions, accidents, etc. in the city;
- cache allocation for video streaming, complaints escalate in real time.

The most significant effect of considering the end-users behavior is that complex systems that have been traditionally split into (smaller) parts, which were then optimized sequentially, now need to be tackled in an integrated fashion. Mobile technology has urged the request of integrated approaches for decision making because of the perception of missing opportunities.

From an optimization perspective, formulating and solving those integrated models is, of course, hard. This is because of (a) volume, (b) velocity, and (c) variety of the data, and also because optimizers are not – in general – trained for that. One answer to this is introducing into the picture some *learning* mechanisms that allow to treat data, often reducing their volume and variety, and to take into account the end-user perspective/behavior.

In the retail context, one needs to predict the sales of a certain product, on a certain shop location, in a certain season, to a certain segment of shoppers, at a certain price. Learning from historical data allows to compute a score associated with these choices and the optimization problem associated with the assortment can be solved only after these scores are computed.

We believe big data applications call for the integration between Machine Learning (ML) [5] and Mathematical Optimization. But, how such an integration should go? And, what about MINLP specifically?

Of course, the easiest integration is already shown in the examples above, where raw data are “crunched” and “prepared” by ML to construct the decision model on which Mathematical Optimization is applied. However, the integration is not restricted to let Machine Learning and Mathematical Optimization work in cascade. Modern ML paradigms like *Deep Learning* [3] are facing more and more complicated structures in which the features (raw data observations) are not kept fixed but are “transformed” within the learning process. Those transformations involve highly nonconvex functions and discrete decisions.

**The role of discrete decisions.** Discrete decisions have been disregarded so far in ML. This is certainly due to the (negative) perception that were not affordable in practical computation (ML has always been concerned with large volumes of data) but it was also related to the fact that the parameters to be learnt were inherently continuous. This is not true anymore in modern paradigms, those that led ML to contribute to the advances in computer vision, signal processing and speech recognition. Moreover, there seems to be large room for using discrete variables to formulate nonconvexities that appear more and more to be crucial in ML (see, e.g., [2]).

**More sophisticated nonlinear models/algorithms.** It is likely there is room for more sophisticated ingredients in Machine Learning both on the function side (predicting functions, generally called “activation” functions) and on the algorithmic side. In addition, the combination of nonlinear functions and discrete decisions could make the learning mechanisms more ambitious. This is true in our running example in retail, where currently the substitution effect of several products in the potential assortment is not directly taken into account by ML in computing the scores. In other words, computing scores for pairs of (substitute) products or for entire assortments (discrete sets) could lead to more sophisticated MINLPs to work with.

We have discussed a few important issues arising in big data optimization, namely

- the change of perspective associated with dealing with the end-users behavior,
- the need of formulating and solving integrated models, and
- the role of (machine) learning.

Optimistically speaking, we see huge opportunities through the interaction between Machine Learning and Mathematical Optimization, especially on the MINLP side.

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## On generalized Benders decomposition and outer approximation for convex chance-constrained problems

GIACOMO NANNICINI

(joint work with Andrea Lodi, Enrico Malaguti, Dimitri Thomopulos)

We study mathematical programs with probabilistic constraints, called *chance-constrained mathematical programming* problems in the literature [2, 8]. Without loss of generality, a chance-constrained mathematical program can be expressed as

$$\text{(CCP)} \quad \max\{cx : \Pr(x \in C_x(w)) \geq 1 - \alpha, x \in X\},$$

where  $w$  is a random variable,  $C_x(w)$  is a set that depends on the realization of  $w$  (the set of probabilistic constraints), and  $X$  is a set that is described by deterministic constraints [8]. The formulation (CCP) allows for two-stage problems with recourse actions, because the sets  $C_x(w)$  can be the projection of higher-dimensional sets. This work discusses the case where recourse actions are allowed and we are interested in the joint probability of  $x \in C_x(w)$ .

We consider the case in which uncertainty can affect all parts of the system of inequalities describing  $C_x(w)$ . We assume that the sample space  $\Omega$  is discrete and finite, i.e.  $\Omega = \{w^i : i = 1, \dots, k\}$ , and all the  $C_x(w^i)$ 's are polyhedra sharing the same recession cone. Under these assumptions, (CCP) can be reformulated as a deterministic mathematical program with integer variables, following a result in [6]. This is accomplished by defining a problem with all the constraints of each of the  $C_x(w^i)$ , and introducing an indicator variable  $z_i$  for each  $w^i$  to activate/deactivate the corresponding constraints.

Unsurprisingly, the size of the problems obtained with the indicator-variable reformulation is unmanageable in most practically relevant situations. However, under relatively mild assumptions it is possible to perform implicit solution of the reformulated problem [7]. The idea is to keep the indicator variables, but avoid the classical on/off reformulation of the constraints that involves them. Then, if cut separation routines for the set  $C_x(w)$  are available, a Branch-and-Cut algorithm

can be applied to the problem  $\max_{x \in X} cx$ , augmented with the indicator variables for the sets  $C_x(w)$  and a constraint to ensure that the scenarios for which the indicator variables are on occur with probability at least  $1 - \alpha$ . This problem is called a master problem. Whenever the solution of the master problem  $\hat{x}$  does not satisfy the chance constraint  $\Pr(\hat{x} \in C_x(w)) \geq 1 - \alpha$ , cuts are generated for the sets  $C_x(w^i)$  for which the corresponding indicator variable  $z_i$  takes the value 1, but  $\hat{x} \notin C_x(w^i)$ . The cuts are then added to the master problem. This basic idea yields an exact algorithm for the original chance-constrained mathematical program. However, the literature mainly focuses on the case where all of the constraints are linear and all the original variables are continuous. The classical decomposition approach for two-stage nonlinear problems is generalized Benders decomposition [5], but it has the drawback of requiring separability and/or knowledge of the problem structure to be practically viable.

In this paper we consider the case where each set  $C_x(w^i)$  is a general closed convex set, and propose a finitely convergent Branch-and-Cut algorithm. The cutting planes that we generate are based on the Projection Theorem and can be obtained as outer approximation cuts [3, 4]. They are linear, as opposed to the possibly nonlinear generalized Benders cuts of [5]. We show that our cuts are a linearization of generalized Benders cuts from a particular choice of dual variables, but our cut generation algorithm is much simpler than the generalized Benders procedure: it can be automated and it has fewer assumptions, more precisely it does not require separability and constraint qualification. While our main focus and computational testing is for the continuous convex case, our algorithm is finitely convergent also in the case where each  $C_x(w^i)$  is a mixed-integer set with a convex continuous relaxation. Generalized Benders decomposition can be seen as a dual approach, while the methodology that we propose is purely primal and automatically generates supporting hyperplanes with little computational overhead, although the inequalities may not be extreme, i.e. they may be obtained as a combination of other valid inequalities.

The main application studied in this work is the scheduling of a hydro valley in a mid-term horizon [1]. We propose a chance-constrained quantile optimization model for this problem that is equivalent to the minimization of the Value-at-Risk. Computational experiments show that our approach is able to solve large instances obtained from data of [1] very effectively, and scales well with  $|\Omega|$ .

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## Multiple linear regression: a mixed integer nonlinear programming approach

JUSTO PUERTO

(joint work with Víctor Blanco, Román Salmerón)

The statistical technique that analyzes the functional relationship between a set of variables  $X_1, \dots, X_d$  is usually called *regression analysis*. It is common to consider that such a dependence is expressed with an equation of the form  $f(X_1, \dots, X_d) = 0$ . The estimation of the function  $f$  that expresses the relationship between the variables is done based on a sample of data. Once the function  $f$  is estimated, such a relationship is used to explain or predict the behavior of one of the variables in terms of the others.

In the linear case, to perform such an estimation of the parameters for a given set of data  $\{x_1, \dots, x_n\} \subset \mathbb{R}^d$ , one tries to find the values  $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_d)$  that minimize some measure of the deviation of the data with respect to the fitting body  $\mathcal{H}(\hat{\beta}) = \{z \in \mathbb{R}^d : \hat{\beta}_0 + \sum_{k=1}^d \hat{\beta}_k z_k = 0\}$ , i.e. the residual. In a general framework, for a given point  $x \in \mathbb{R}^d$ , we define the *residual* of a model as a mapping  $\varepsilon_x : \mathbb{R}^{d+1} \rightarrow \mathbb{R}_+$ , that maps any  $\beta = (\beta_0, \dots, \beta_d) \in \mathbb{R}^{d+1}$ , into a measure  $\varepsilon_x(\beta)$  that represents how much deviates the fitting of the model, with those parameters, from the observation  $x$ . The larger this measure, the worse the fitting for such a point  $x$ . The final goal of a regression model for a given set of points  $\{x_1, \dots, x_n\} \subseteq \mathbb{R}^d$  is to find the fitting body minimizing a globalizing function,  $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$ , of the residuals of all the points.

In this talk we present a new framework for multiple linear regression that allows the decision maker/statistician to decide within a wide family of residuals and criteria [8] which is the “best” for a given sample of data. One of the main highlights of our proposal is the use of modern mathematical programming tools to solve the MINLP problems which are involved in the computation of the estimated parameters of the fitting models. The optimization models for those problems range from continuous convex programming to mixed integer nonlinear programming through linear programming. Many of the formulations described in this paper have been implemented in R in order to be available for statisticians and practitioners.

The new framework for multiple regression proposed in this paper can be easily combined with the mathematical programming techniques for feature selection, to “choose” a fixed number of variables to explain the dependence between a set of variables [3], with classification schemes [2], or with linear constrained regression models, where the coefficients are required to fulfill a set of linear equations/inequalities.

The description of such a family of combinations residuals-criteria needs to define a generalized measure of the goodness of the fitting for the different models. Thus, a new measure is provided in order to make the comparison meaningful.

One of the important novelties of the approach is that errors are measured as shortest distances, based on a norm, between the given data and the fitting surface. This makes the fitting geometrically invariant. We remark that this framework also subsumes as a particular case the standard linear regression methods that consider residuals based on vertical distances; as well as most of the particular cases of linear regression for vertical distances but different aggregation criteria described in the literature, as  $\ell_p$  regression ( $\ell_p$ -norm criterion), least quantile of squares [10, 3], least trimmed sum of squares [9, 1], etc. The use of nonstandard residuals is not usual in the literature although orthogonal ( $\ell_2$ ) residuals have been already used, see e.g. Euclidean Regression [4] or Total Least Squares Regression [7], mainly applied to bidimensional data. Quoting the reasons for that fact given by Giloni and Padberg in [6]: “we have left out a summary of linear regression models using the more general  $\ell_\tau$ -norms with  $\tau \notin \{1, 2, \infty\}$  for which the computational requirements are considerably more burdensome than in the linear programming case (as they generally require methods from convex programming where machine computations are far more limited today).”

Summarizing we introduce a new framework for multivariate linear regression together with an alternative generalized coefficient of determination. We analyze the classical multivariate linear regression methods under the new framework: new mathematical programming models for adequate aggregation criteria and residuals are provided for: 1) least sum of squares; 2) least absolute deviation; 3) least quantile of squares and 4) least trimmed of squares regression. Next, we present new methods for the multivariate linear regression problem assuming that the residuals are measured as the smallest norm-based distance between the sample data and the linear fitting body for polyhedral and  $\ell_p$  norms. Finally, we report computational experiments for synthetic data and for the classical data set given in [5].

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## Active set methods for convex quadratic problems with simple bound constraints

FRANZ RENDL

(joint work with P. Hungerländer)

We consider the following simple optimization problem:

$$\min \frac{1}{2}x^T Qx + q^T x \text{ such that } x \leq b.$$

The symmetric  $n \times n$  matrix  $Q$  is assumed to be positive definite. This problem is well known to be tractable. The objective function is denoted by  $J(x)$ . A vector  $x$  together with multipliers  $\alpha$  is optimal if and only if the following conditions hold:

$$Qx + q + \alpha = 0; \alpha \circ (b - x) = 0, \alpha \geq 0, b - x \geq 0.$$

We use  $a \circ b$  to denote the elementwise product of vectors  $a$  and  $b$ . Suppose that  $A \subseteq N := \{1, \dots, n\}$  is selected to contain the active variables, meaning that  $x_A = b_A$ . The complement of  $A$  is denoted by  $I := N \setminus A$ . Setting  $\alpha_I = 0$  insures that the complementarity condition  $\alpha \circ (b - x) = 0$  is satisfied. We call the pair  $(x, \alpha)$  the subspace solution to  $A$  if

$$Qx + q + \alpha = 0, x_A = b_A, \alpha_I = 0$$

and write  $[x, \alpha] = KKT(A)$  for short. It solves the original problem if  $x_I \leq b_I$  and  $\alpha_A \geq 0$ . Bergounioux et al [1] introduced the following simple active set iterations.

Start with  $A \subseteq N$ , compute  $[x, \alpha] = KKT(A)$ . If the solution is optimal ( $x \leq b, \alpha \geq 0$ ) then stop, otherwise continue with new set

$$(1) \quad B \leftarrow \{i : x_i > b_i\} \cup \{i : \alpha_i > 0\}.$$

Hintermüller et al [2] have shown that this iterative scheme can be interpreted as a semismooth Newton method, applied to an appropriately chosen system of equations. They also show global convergence if  $Q$  is an  $M$ -matrix, but it is known that this iterative scheme may cycle in general.

In this talk we present two variants of the method, that insure global convergence for any  $Q \succ 0$ .

**Primal feasible iterates:** In the first variant, we maintain primal feasible active sets  $A$ , i.e.  $x = KKT(A)$  will satisfy  $x \leq b$ . This is achieved as follows. While  $KKT(A)$  has components  $x_i > b_i$  we keep adding these indices to  $A$  and iterate this process. Clearly this will terminate with a final active set  $A$  having  $KKT(A) \leq b$ .

Let us consider two consecutive primal feasible sets  $A$  and  $B$  obtained this way with  $x = KKT(A)$ ,  $y = KKT(B)$ .

If  $J(y) < J(x)$  we continue with  $B$ . Otherwise, if  $|A| = 1$ , i.e.  $A$  contains only one active index, say  $j$ , we see that having  $x_j = b_j$  is not optimal, hence  $j$  will be inactive, and we have reduced the dimension of the problem by one, which we now solve by induction.

The final case  $J(y) \geq J(x)$ ,  $|A| > 1$  is also handled by recursion. Here we select a nonempty set  $A_0 \subset A$  such that  $KKT(A)$  is feasible but not optimal on  $A_0$ . This is always possible. We solve the problem with  $x_{A_0} = b_{A_0}$ ,  $x \leq b$  (with less constraints) by recursion, and get the optimal active set  $B_0$ . We continue the algorithm with the new active set  $B \leftarrow A_0 \cup B_0$ . This ensures strict decrease of objective function values, and hence finite termination of the algorithm. For details we refer to [3].

**Red-green Iterates:** In the second variant we allow infeasible iterates and maintain the following property during each iteration: We have the configuration  $(A, [x, \alpha], u)$  with

$$Qx + q + \alpha = 0, \quad x_A = b_A, \quad u = \min\{x, b\}.$$

Moreover if  $x \leq b$  then  $[x, \alpha] = KKT(A)$ .

A configuration is called green if  $[x, \alpha] = KKT(A)$  and red otherwise. Therefore primal feasible iterates are always green. We do not require primal feasibility but insure consecutive iterates to have **projections**  $u$  and  $v$  with  $J(v) < J(u)$ .

We first consider the update (1) with subspace solution  $[y, \beta] = KKT(B)$  and  $v = \min\{y, b\}$ . We declare this update successful if  $J(v) < J(u)$ . In this case the new configuration is  $(B, [y, \beta], v)$  green.

Otherwise we need to modify the update (1) to insure global convergence. We distinguish two cases:

- $x$  is strictly feasible:  $\forall i \notin A : x_i < b_i$ . We set  $A^+ \leftarrow A \setminus j$  with  $j \in A$ ,  $\alpha_j < 0$
- $x$  not strictly feasible:  $\exists i \notin A : x_i \geq b_i$ . Here we set  $A^+ \leftarrow A \cup \{i \notin A, x_i \geq b_i\}$ .

In the first case, we start with a green configuration and we can show that the new configuration yields a strict decrease of objective values. In [4] it is shown that the number of consecutive red configurations is bounded by  $n$  with nonincreasing objective values. Finally, between two green configurations there is strict decrease of the objective values, leading to finite termination.

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## Exploiting Linear Symmetry in Integer Convex Optimization using Core Points?

ACHILL SCHÜRMAN

(joint work with Katrin Herr and Thomas Rehn)

For many years it has been known that symmetry in integer linear and convex optimization leads often to difficult problem instances. Standard approaches like branching usually work particularly poorly when large symmetries are present. Nevertheless, in the past decade several authors have suggested methods to use symmetry for certain special classes of problems (see for instance [5, 6, 7, 8]). The two commercial solvers **Gurobi** and **CPLEX** by now can successfully exploit special symmetries (generated by transpositions of variables).

**Linear symmetries.** In an ongoing project (supported currently by DFG Grant SCHU 1503/6-1) we have been working on exploiting symmetry in polyhedral computations (see [10] for an overview). In contrast to previous approaches, we are following in particular the idea to make use of the rich geometry coming with a linear (respectively affine) symmetry group. Here, considering linear symmetries is no restriction in practice, since these are the only symmetries we can compute practically anyway for a given problem (see [2]). Among other things, our software **SymPol** [11] can automatically compute the linear symmetry group of a polyhedron given by vertices or linear inequalities only.

**Integer Convex Optimization Problems.** We consider the class of problems

$$(1) \quad \min_{x \in \mathbb{Z}^n} c^t x \quad \text{such that} \quad x \in \mathcal{F} \subseteq \mathbb{R}^n,$$

where  $\mathcal{F}$  denotes some kind of convex “feasible set”. The *integral linear symmetry group* of problem (1) is defined as the (finite) group  $\Gamma \leq \text{GL}_n(\mathbb{Z}) = \{g \in \mathbb{Z}^{n \times n} : |\det g| = 1\}$  preserving the problem when acting on the  $x$  variables, that is, if  $g\mathcal{F} = \mathcal{F}$  and  $c^t(gx) = c^t x$  for all  $g \in \Gamma$  and for all  $x \in \mathcal{F}$ .

**Linear vs. Permutation Symmetries.** Usually, in integer optimization problems, researchers have restricted their attention to permutation symmetries on the variables so far. These are easier to compute or often known a priori from the problem or model used. In his thesis [9] Thomas Rehn reports on a study of permutation symmetries of problem instances from MIPLIB 2010. It turns out that 209 of the 357 instances have non-trivial symmetry, many of them on all or almost all of the variables and sometimes of surprising large order. Among the 50 smallest instances (with less than 1500 variables) Rehn also computed the linear symmetry groups. It turned out that six of the instances have linear symmetries, which do not come from (signed) permutation matrices. So far it is unclear where these symmetries come from! Further studies of these unexpected  $GL_n(\mathbb{Z})$  symmetries are needed.

**Fixed Spaces and Core Points.** In a  $\Gamma$ -symmetric convex optimization problem without integrality constraints it is possible to reduce the dimension of the problem by intersecting with the fixed space  $\{x \in \mathbb{R}^n : \Gamma x = x\}$  of the linear group  $\Gamma$ . Convexity guarantees that the optimization problem has a solution in the fixed space if it has a solution at all.

To make use of integral linear symmetries we define and study a discrete analogue of the fixed space. We say  $z \in \mathbb{Z}^n$  is a *core point* of  $\Gamma \leq GL_n(\mathbb{Z})$  if the convex hull  $\text{conv}(\Gamma z)$  of its orbit  $\Gamma z$  contains no integral points other than those from the orbit, that is, if

$$\text{conv}(\Gamma z) \cap \mathbb{Z}^n = \Gamma z.$$

The value of this concept lies in the fact that any  $\Gamma$ -invariant convex integer optimization problem (of the form (1)) which has a solution, attains its optimal value at one of the core points. Thus when solving a  $\Gamma$ -invariant integer convex optimization problem, one can restrict the problem to the core points of  $\Gamma$ . Note that core points do not rely on a specific problem instance. Given a linear group  $\Gamma$  one can therefore try to classify or approximate core points and then use this geometric information for solving any problem instance having  $\Gamma$ -symmetries.

**First computational experiments.** As a first class of examples, we considered direct products of symmetric groups in [1]. We showed that the core points are 0/1-vectors, up to integrality preserving translations of the fixed space. We have used this information in conjunction with a naive enumeration algorithm to beat the two state-of-the-art professional solvers **Gurobi** and **CPLEX** on a series of “cooked up” small dimensional problems with such symmetry groups. With a reformulation idea we also were able to solve a MIPLIB 2010 problem that was previously unsolved (instance `toll-like`).

**Developing a theory.** In [3] we took a first step in direction of a systematic classification of core points. For that we restricted ourselves to the study of transitive permutation groups. This is a first necessary building block for future work, since more general permutation groups are contained in a direct product of transitive groups. A quite useful **theorem** we discovered shows that core points are

always near invariant subspaces of a given linear group  $\Gamma$ . From basic representation theory it is known that  $\mathbb{R}^n$  decomposes into a direct sum of  $\Gamma$ -invariant irreducible subspaces. For transitive groups one of them is the one dimensional space spanned by the all-ones-vector  $\mathbb{1}$ . In case its orthogonal complement can not be decomposed into more than one invariant subspace (that is, if the complement is  $\mathbb{R}$ -irreducible), our theorem implies that there exist only finitely many core points up to integral translations of the fixed space (translations by multiples of  $\mathbb{1}$ ). By a result of Cameron (dating back to 1972) these groups are precisely the 2-homogeneous groups. For such groups, using a database of transitive permutation groups in GAP, we classified all core points up to  $n = 12$ .

We **conjecture** that for all other transitive permutation groups, there exist infinitely many core points, up to integral translations of the fixed space. So far we have proved the conjecture for groups  $\Gamma$  with irrational invariant subspaces. For groups having rational invariant subspaces we were able to give a prove only in case when the groups are imprimitive. The conjecture therefore remains open for primitive permutation groups with rational invariant subspaces only. Using a computer in conjunction with some developed criteria we checked the conjecture for this remaining class of groups up to  $n = 127$ . It turns out that latter groups are well suited to create difficult low dimensional instances for commercial solvers like Gurobi and CPLEX. In his thesis, Rehn reports on a series of feasibility tests for symmetric simplices. Whereas commercial solvers appear to be unable to solve such problems, knowing their symmetry group and the invariant subspace structure, allows one to solve these problems for instance with a suitable branching strategy (see [9] for details).

**Conclusion.** Subsuming we can say that the core point concept has quite some potential. It has been shown that it can be used successfully on specific problems. Even the geometry of core points of linear groups with infinite core sets (up to fixed space translations) can be exploited. However, at this point, not only more advanced algorithms are missing, but also many fundamental theoretical questions are still open. General  $GL_n(\mathbb{Z})$  symmetries and their core points are not well understood at this point. There is still a lot to be done and to be discovered!

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## The vertex separator problem

RENATA SOTIROV

(joint work with Franz Rendl)

The vertex separator problem (VSP) for a graph is to find the subset of vertices of small cardinality, that is called vertex separator, whose removal breaks the graph into two disconnected subsets.

Some families of graphs are known to have small vertex separators. Lipton and Tarjan [2] provide a polynomial time algorithm which determines a vertex separator in  $n$ -vertex planar graph of size  $O(\sqrt{n})$ . Their result was extended to some other families of graphs such as graphs of fixed genus [3]. It is also known that trees, 3D-grids and meshes have small separators. However, there are existing graphs that do not have small separators such as hypercubes and expander graphs.

The VSP problem arises in many different fields such as VLSI design, clustering, machine learning, bioinformatics, etc. Finding vertex separators of small size is an important problem in communications network and finite element methods. The VSP also plays a role in divide-and-conquer algorithms for minimizing the work involved in solving system of equations, see e.g., [3, 4].

The vertex separator problem is related to the following graph partition problem. Let  $G = (V, E)$  be an undirected graph with vertex set  $V$ , where  $|V| = n$  and edge set  $E$ . We denote by  $A$  be the adjacency matrix of  $G$ . For given  $m = (m_1, m_2, m_3)^T$ ,  $\sum_{i=1}^3 m_i = n$ , we consider the following minimum cut (MC) problem:

$$\text{OPT}_{\text{MC}} := \min \left\{ \sum_{i \in S_1, j \in S_2} a_{ij} : (S_1, S_2, S_3) \text{ partitions } V \text{ and } |S_i| = m_i, \forall i \right\}.$$

This problem asks to find a vertex partition  $(S_1, S_2, S_3)$  with specified cardinalities, such that the number of edges joining vertices in  $S_1$  and  $S_2$  is minimized. It is clear that if  $\text{OPT}_{\text{MC}} = 0$  for some  $m = (m_1, m_2, m_3)$  then  $S_3$  separates  $S_1$  and  $S_2$ . On the other hand,  $\text{OPT}_{\text{MC}} > 0$  shows that no separator  $S_3$  for the cardinalities specified in  $m$  exists. Our approach is to compute lower bounds of the MC problem by solving semidefinite programming (SDP) problems of increasing complexity, which leads us to lower bounds on the size of the separator.

We consider here several semidefinite programming relaxations for the minimum cut problem. The following simple semidefinite program is our starting SDP relaxation:

$$\begin{aligned}
 (SDP_1) \quad & \min \quad \text{tr}(AY_{12}) \\
 \text{s.t.} \quad & \text{tr}(Y_i) = m_i, \text{tr}(JY_i) = m_i^2, \quad i = 1, 2 \\
 & \text{diag}(Y_{12}) = 0, \text{tr}(J(Y_{12} + Y_{12}^T)) = 2m_1m_2 \\
 & Y = \begin{pmatrix} Y_1 & Y_{12} \\ Y_{12}^T & Y_2 \end{pmatrix}, \quad y = \text{diag}(Y), \quad \begin{pmatrix} Y & y \\ y^T & 1 \end{pmatrix} \succeq 0,
 \end{aligned}$$

where  $J$  and  $e$  denote all-ones matrix and all-ones vector respectively, and the ‘diag’ operator maps an  $n \times n$  matrix to the  $n$ -vector given by its diagonal. The SDP relaxation  $(SDP_1)$  has  $3n + 6$  linear equality constraints. We prove that the resulted SDP bound is stronger than the known eigenvalue bound for the MC by Helmberg et al., [1] that can be expressed as the optimal solution of the semidefinite program with matrices of order  $3n$ .

To tighten  $(SDP_1)$  we first add elementwise nonnegativity constraints on support, and then the following set of inequalities

$$\begin{aligned}
 1 - (y_i + y_j + y_{n+i} + y_{n+j}) + Y_{i,j} + Y_{i,n+j} + Y_{j,n+i} + Y_{n+i,n+j} &\geq 0, \quad \forall i < j \\
 y_j - Y_{i,j} - Y_{n+i,j} &\geq 0, \quad y_{n+j} - Y_{i,n+j} - Y_{n+i,n+j} \geq 0 \quad \forall i \neq j \\
 1 - y_i - y_{n+i} - y_j + Y_{i,j} + Y_{n+i,j} &\geq 0 \\
 1 - y_i - y_{n+i} - y_{n+j} + Y_{i,n+j} + Y_{n+i,n+j} &\geq 0 \quad i \neq j, \quad \forall i, j \in V.
 \end{aligned}$$

In order to further strengthen resulted SDP relaxation, we add the following facet defining inequalities of the boolean quadric polytope (BQP), see e.g., [5],

$$\begin{aligned}
 0 &\leq Y_{i,j} \leq Y_{i,i} \\
 Y_{i,i} + Y_{j,j} &\leq 1 + Y_{i,j} \\
 Y_{i,k} + Y_{j,k} &\leq Y_{k,k} + Y_{i,j} \\
 Y_{i,i} + Y_{j,j} + Y_{k,k} &\leq Y_{i,j} + Y_{i,k} + Y_{j,k} + 1.
 \end{aligned}$$

Our preliminary numerical results show that our strongest SDP relaxation provides tight bounds of the MC problem for graphs with less than 200 vertices. For those graphs we find vertex separators of small size. For larger graphs with less than 500 vertices, we obtain good bounds for the minimum cut problem which lead to good bounds on the size of the separator. To compute feasible solutions we apply a variant of Kerningham-Lin heuristics.

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## MINLP from a discrete geometry point of view

FRANK VALLENTIN

A large class of optimization problems in discrete geometry is concerned with the optimal distribution of a finite number of points  $X = \{x_1, \dots, x_N\}$  on a compact manifold  $M$ . There are many possibilities to optimize the quality of such a geometric configuration  $X$ : One can maximize the packing density — which is by far the best-studied example. Other important geometric optimization problems in discrete geometry are minimizing potential energy or minimizing covering density.

All these optimization problems have the flavor of a binary optimization problem (with a nonlinear objective function): For every point  $x \in M$  one has to make the binary decision whether  $x$  belongs to the finite set  $X$  or not. Here, in the geometric setting, one has infinitely many binary decisions to make, whereas in standard MINLP, optimization problems only involve finitely many binary decision variables. One approach to solve such standard MINLPs is by employing Lasserre’s hierarchy from polynomial optimization.

An example, which can be used to model packing problems in discrete geometry, is finding the independence number  $\alpha(G)$  of a finite graph  $G = (V, E)$ . One can equivalently reformulate the problem of finding  $\alpha(G)$  as a polynomial optimization problem. Then Lasserre’s hierarchy gives an equivalent convex optimization problem. Following Laurent [6], the  $t$ -th step of Lasserre’s hierarchy is:

$$\text{las}_t(G) = \max \left\{ \sum_{x \in V} y_{\{x\}} : y \in \mathbb{R}_{\geq 0}^{I_{2t}}, y_\emptyset = 1, M_t(y) \text{ is positive semidefinite} \right\},$$

where  $I_t$  is the set of all independent sets with at most  $t$  elements and where  $M_t(y) \in \mathbb{R}^{I_t \times I_t}$  is the moment matrix defined by the vector  $y$ : Its  $(J, J')$ -entry equals

$$(M_t(y))_{J, J'} = \begin{cases} y_{J \cup J'} & \text{if } J \cup J' \in I_{2t}, \\ 0 & \text{otherwise.} \end{cases}$$

The first step in Lasserre’s hierarchy coincides with the  $\vartheta'$ -number, the strengthened version of Lovász  $\vartheta$ -number which is due to Schrijver. Furthermore the hierarchy converges to  $\alpha(G)$  after at most  $\alpha(G)$  steps:

$$\vartheta'(G) = \text{las}_1(G) \geq \text{las}_2(G) \geq \dots \geq \text{las}_{\alpha(G)}(G) = \alpha(G).$$

Lasserre [5] showed this convergence in the general setting of hierarchies for 0/1 polynomial optimization problems by using Putinar’s Positivstellensatz and the flat extension theorem of Curto and Fialkow. Laurent [6] gave an elementary proof using combinatorial moment matrices.

In the talk I proposed the following three-step strategy to solve or to give rigorous approximations of optimization problems in discrete geometry:

**Step 1:** *Convexify the problem by setting up an infinite-dimensional version of Lasserre's hierarchy.*

Again as a principal example we consider the problem of finding the independence number of a graph but now with potentially infinitely many vertices. We consider topological packing graphs where vertices which are close are adjacent, and where vertices which are adjacent will stay adjacent after small enough perturbations. A concrete example are *distance graphs*  $G = (V, E)$  where  $(V, d)$  is a metric space, and where there exists  $D \subseteq (0, \infty)$  such that  $x$  and  $y$  are adjacent precisely when  $d(x, y) \in D$ . Formally, a graph whose vertex set is a Hausdorff topological space is called a *topological packing graph* if each finite clique is contained in an open clique. An *open clique* is an open subset of the vertex set where every two vertices are adjacent.

The  $t$ -th step of the generalized hierarchy of a topological packing graph is

$$\text{las}_t(G) = \sup \left\{ \lambda(I_{=1}) : \lambda \in \mathcal{M}(I_{2t})_{\geq 0}, \lambda(\{\emptyset\}) = 1, A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0} \right\},$$

where  $\mathcal{M}(I_{2t})_{\geq 0}$  denotes the cone of positive Radon measures on  $I_{2t}$ , and where condition  $A_t^* \lambda \in \mathcal{M}(I_t \times I_t)_{\geq 0}$  says that measure  $\lambda$  satisfies a moment condition, see [4] for the technical details.

We have a nonincreasing chain

$$\text{las}_1(G) \geq \text{las}_2(G) \geq \dots \geq \text{las}_{\alpha(G)-1}(G) \geq \text{las}_{\alpha(G)}(G) = \text{las}_{\alpha(G)+1}(G) = \dots,$$

which stabilizes after  $\alpha(G)$  steps, and specializes to the original hierarchy if  $G$  is a finite graph. Each step gives an upper bound for  $\alpha(G)$  because for every independent set  $S$  the measure

$$\lambda = \sum_{Q \in I_{2t}: Q \subseteq S} \delta_Q, \quad \text{where } \delta_Q \text{ is the delta measure at } Q,$$

is a feasible solution for  $\text{las}_t(G)$  with objective value  $|S|$ . In [4] it is shown that we have also have finite convergence after at most  $\alpha(G)$  steps,  $\alpha(G) = \text{las}_{\alpha(G)}$ . So the generalized hierarchy provides a convex reformulation for packing problems on compact manifolds.

Computing higher steps in this hierarchy is computationally intractable. So we aim to compute the first steps. These are infinite-dimensional semidefinite programs.

**Step 2:** *Simplify the infinite-dimensional semidefinite programs using the symmetry of the manifold.*

This gives a simpler semidefinite program in the Fourier space determined by the manifold. Simpler means that the semidefinite program has some block-diagonal form (although it stays being infinite-dimensional). The basic theory underlying this symmetrization process is explained in [1].

**Step 3:** *Solve the simplified infinite-dimensional semidefinite program on a computer by discretizing the function space.*

Here discretizing by using polynomials in some given finite-dimensional vector space has been a successful choice. In view of getting reliable numerical solutions, one has to use well-conditioned polynomial basis functions in this step.

**Results.** This three-step strategy has been worked out successfully for several geometric packing problems. We frequently could improve the known upper bounds. In the talk I reported on improved bounds for unary and binary sphere packings [3], regular pentagon packings in the plane [7], and translative packings of regular tetrahedra in three-dimensional space [2].

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## Extended and Embedding Formulations for MINLP

JUAN PABLO VIELMA

### 1. INTRODUCTION

We consider strong Mixed Integer Programming (MIP) formulations for a disjunctive constraint of the form

$$(1) \quad x \in \bigcup_{i=1}^n C_i$$

where  $\{C_i\}_{i=1}^n \subseteq \mathbb{R}^d$  is a finite family of compact convex sets. MIP formulations for (1) can be divided into two classes depending on their strength and types of auxiliary variables. The first class corresponds to extended formulations that use both 0-1 and continuous auxiliary variables. Standard versions of such extended formulations have sizes that are linear on appropriate size descriptions of the convex sets (e.g. number of linear, quadratic or conic constraints) and have continuous relaxations with extreme points that naturally satisfy the integrality constraints on the 0-1 variables (such formulations are usually denoted *ideal* and

are as strong as possible). Extended formulations for polyhedral sets have been introduced by Balas, Jeroslow and Lowe (e.g. see [15, Section 5]), for conic representable sets by Ben-Tal, Helton, Nemirovski and Nie [1, 7] and for sets described through non-linear inequalities by Ceria, Merhotra, Soares and Stubs [3, 10]. The second class corresponds to non-extended formulations that only use the 0-1 variables that are strictly necessary for a valid formulation. Standard versions of such non-extended formulations are also linear sized, but are often significantly weaker than their extended counterparts. Non-extended formulations include big-M type constraints and ad-hoc formulations for specially structured polyhedral sets (e.g. see [15, Section 6] for the polyhedral case and [2, 4, 5, 12] for sets described by non-linear inequalities). In this talk we consider aspects of both extended and non-extended formulations of unions of convex sets as described in the sequel.

## 2. EXTENDED FORMULATIONS

While extended formulations for unions of convex sets are usually too expensive to be used directly in practice a different kind of extended formulation can significantly improve the performance of LP-based algorithms for (convex) Mixed Integer Nonlinear Programming (MINLP). Such algorithms work by approximating (convex) nonlinear constraints with polyhedral relaxations. These algorithms are extremely effective when few linear inequalities are enough to get good approximations of the nonlinear constraints. However, when a large number of linear inequalities are needed they can lag behind NLP-based algorithms. A recent trend to resolve this issue is to use lifted approximations of the nonlinear constraints, that is, to approximate these constraints as the projection of a polyhedron. Such lifted approximations are often constructed through regular polyhedral approximations of extended formulations of the nonlinear constraints. Examples of such extended formulations are those proposed by [6, 11] for separable nonlinear constraints and by [14] for conic quadratic constraints. Using such extended formulations or lifted approximations has been shown to provide a significant computational advantage, but so far their applicability is restricted to specially structured nonlinear constraints. In this talk we show how the conic extended formulations for unions of convex sets from [1, 7] can be used to expand the applicability of lifted approximations in LP-based algorithms for MINLP.

## 3. NON-EXTENDED EMBEDDING FORMULATIONS

A common feature of MIP formulations for unions of convex sets is the use of  $n$  0-1 variables that are constrained to add up to one. However, in the polyhedral setting different uses of 0-1 variables can lead to non-extended formulations that are ideal, smaller than the smallest extended counterpart and provide a significant computational advantage [13]. In [16] we introduce a systematic procedure to construct non-extended formulations for unions of polyhedra, which have a flexible use of 0-1 variables. The following definition is a straightforward extension of such procedure to unions of compact convex sets.

**Definition 1** (Embedding Formulations). Let  $\mathcal{C} := \{C_i\}_{i=1}^n$  be a family of compact convex sets in  $\mathbb{R}^d$ ,  $H := \{h^i\}_{i=1}^n \subseteq \{0, 1\}^k$  be such that  $h^i \neq h^j$  and  $Q \subseteq \mathbb{R}^{d+k}$  be a closed convex set. We say  $(Q, H)$  is a formulation for  $\bigcup_{i=1}^n C_i$  if and only if

$$(x, h) \in Q \cap (\mathbb{R}^d \times \mathbb{Z}^k) \quad \Leftrightarrow \quad \exists i \in \{1, \dots, n\} \text{ s.t. } h = h^i \wedge x \in C_i.$$

An ideal formulation can be obtained by taking  $Q$  equal to

$$Q(\mathcal{C}, H) := \text{conv} \left( \bigcup_{i=1}^n C_i \times \{h^i\} \right).$$

If  $k = n$  and  $h^i = e^i$ , the  $i$ -th unit vector, we obtain a formulation with the traditional use of integer variables and if  $n = 2^k$  and  $H = \{0, 1\}^k$  we obtain a so-called logarithmic formulation (e.g. [15]). Following [17], we refer to these two choices of  $H$  as unary and binary encodings respectively as they can be interpreted as the corresponding encoding of the choice among the  $C_i$ . Furthermore, because for polyhedral  $C_i$  and the unary encoding,  $Q(\mathcal{C}, H)$  (and sometimes  $\bigcup_{i=1}^n C_i \times \{h^i\}$ ) is usually denoted the Cayley Embedding of  $\{C_i\}_{i=1}^n$  (e.g. [8, 9]), we refer to  $(Q(\mathcal{C}, H), H)$  as an *embedding formulation* of (1).

If  $C_i$  are rational polyhedra we can obtain a non-extended ideal formulation by simply constructing  $Q(\mathcal{C}, H)$ . However, the number of inequalities of  $Q(\mathcal{C}, H)$  can easily be exponential on the number of inequalities of the  $C_i$ . In fact, it is well known that for the unary encoding  $Q(\mathcal{C}, H)$  contains the Minkowski sum of  $\{C_i\}_{i=1}^n$  through an appropriate affine section (e.g. [8, 9]). This can make the unary encoded  $Q(\mathcal{C}, H)$  large even if  $\text{conv}(\bigcup_{i=1}^n C_i)$  is small. In this talk we review some results from [16] that show that in such cases the size of  $Q(\mathcal{C}, H)$  can be significantly reduced by using specially selected binary encodings.

While the containment of the Minkowski sum can be a burden in the polyhedral setting, it can also be used to give precise descriptions the unary encoded  $Q(\mathcal{C}, H)$  for some non-polyhedral sets  $C_i$ . We illustrate such approach through several examples that generalize results from [2, 4, 5]. We also use this approach to show that even if sets  $C_i$  are described by linear and convex quadratic inequalities it may happen that  $Q(\mathcal{C}, H)$  cannot be described by a finite number of polynomial inequalities.

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## An FPTAS for Minimizing Indefinite Quadratic Forms over Integers in Polyhedra

ROBERT WEISMANTEL

(joint work with R. Hildebrand, K. Zemmer)

Consider the problem

$$(1) \quad \min\{f(x) : x \in P \cap \mathbb{Z}^n\}$$

for  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $P = \{x \in \mathbb{R}^n : Ax \leq b\}$ ,  $A \in \mathbb{Z}^{m \times n}$ , and  $b \in \mathbb{Z}^m$ . We use the words *size* and *binary encoding length* synonymously. The size of  $P$  is the sum of the sizes of  $A$  and  $b$ . We assume throughout this talk that  $P$  is bounded. We say that Problem (1) can be solved in polynomial time if in time bounded by a polynomial in the size of its input, we can either determine that the problem is infeasible, or we can find a feasible minimizer.

The main focus of this talk is Problem (1) with  $f(x) = x^T Q x$ , where  $Q \in \mathbb{Z}^{n \times n}$  is a symmetric matrix. Note that if  $Q$  is not symmetric, then we can replace it by  $Q' = \frac{1}{2}Q + \frac{1}{2}Q^T$ , which is symmetric and satisfies  $x^T Q x = x^T Q' x$ . The input size of Problem (1) with  $f(x) = x^T Q x$  is the sum of the sizes of  $P$  and  $Q$ . For  $n \leq 2$ , the problem is polynomial time solvable [5]. When  $Q$  is positive semi-definite,  $f(x)$  is convex, whereas it is concave when  $Q$  is negative semi-definite. In the former case, Problem (1) with fixed  $n$  and bounded  $P$  can be solved in polynomial time by [4], whereas in the latter case by [3].

The computational complexity of integer polynomial optimization in fixed dimension was surveyed in [2], and they develop an FPTAS for maximizing non-negative polynomials over integer points in a polytope, respectively.

We use a notion of approximation that is common in combinatorial optimization and is akin to the maximization version used in [2] for maximizing non-negative polynomials over polyhedra, except here, we extend the notion to allow for the objective to take negative values.

**Definition.** Let  $x_{\text{opt}}$  be an optimal solution to Problem (1) and let  $\epsilon > 0$ . We say that  $x_\epsilon$  is an  $\epsilon$ -approximate solution to Problem (1) if  $x_\epsilon$  is feasible and one of the following hold:

- (1)  $f(x_{\text{opt}}) > 0$  and  $f(x_\epsilon) \leq (1 + \epsilon)f(x_{\text{opt}})$ ,
- (2)  $f(x_{\text{opt}}) < 0$  and  $f(x_\epsilon) \leq \frac{1}{1+\epsilon}f(x_{\text{opt}})$ ,
- (3)  $f(x_{\text{opt}}) = 0$  and  $f(x_\epsilon) = f(x_{\text{opt}})$ .

We say an algorithm for Problem (1) is a *fully polynomial-time approximation scheme* if for any  $\epsilon > 0$ , in polynomial time in  $\frac{1}{\epsilon}$  and the size of the input, the algorithm correctly determines whether the problem is feasible, and if it is, outputs an  $\epsilon$ -approximate solution  $x_\epsilon$ .

In order to develop an FPTAS for classes of nonlinear functions to be minimized over integer points in polyhedra, we propose a framework that combines the techniques of Papadimitriou and Yannakakis [1] with ideas similar to those commonly used to derive certificates of positivity for polynomials over semialgebraic sets. Generally speaking, in the latter context one is given a finite number of “basic polynomials”  $f_1, \dots, f_m$  which are known to be positive over the integers in a polyhedron  $P$ . A sufficient condition to prove that another polynomial  $f$  is positive over  $P \cap \mathbb{Z}^n$  is to find a decomposition of  $f$  as a sum of products of a *sum of squares* (SOS) polynomial and a basic function  $f_i$ . A polynomial  $p(x)$  is SOS if there exist polynomials  $q_1(x), \dots, q_m(x)$  such that  $p(x) = \sum_{i=1}^m q_i^2(x)$ .

We would like to use a similar approach to arrive at an FPTAS. Again we work with classes of “basic functions”. Then, for a given  $f$ , we try to detect a decomposition of  $f$  as a finite sum of products of a so-called “sliceable function” and a basic function  $f_i$ . Roughly speaking, sliceable functions — thanks to the result of [1] — can be approximated by subdividing the given polyhedron.

For instance, the set of all convex functions presented by a first order oracle that are nonnegative over  $P \cap \mathbb{Z}^n$  could serve as a class of basic functions, because we can solve Problem (1) for any member in the class in polynomial time when  $n$  is fixed. The nonnegativity assumption implies sign-compatibility, which is a necessary property of the set of basic functions that will be discussed in this talk. Another example is the set of all concave functions presented by an evaluation oracle that are nonnegative over  $P \cap \mathbb{Z}^n$ . The same property holds true in this case. These two examples demonstrate that we consider not only polynomials  $f_i$ , but also more general classes of basic functions. In fact, this is key to tackle the quadratic optimization problem. For example, we can decompose the polynomial  $x^2 + y^2 - z^2$  as the product of two non-polynomial functions: a basic function  $\sqrt{x^2 + y^2} - |z|$

and a sliceable function  $\sqrt{x^2 + y^2} + |z|$ . Our technique also applies, for instance, to the Motzkin polynomial, but to functions  $f$  that are not polynomials as well.

We explain axiomatically what we mean by basic and sliceable functions. As a consequence of our technique we easily derive the following result that in the optimization community was an open question for several years.

**Theorem.** Let  $Q \in \mathbb{Z}^{n \times n}$  be a symmetric matrix and let  $n$  be fixed. Then there is an FPTAS for Problem (1) with  $f(x) = x^T Q x$  in the following cases:

- (1)  $Q$  has at most one negative eigenvalue;
- (2)  $Q$  has at most one positive eigenvalue.

We also sketch a proof for this theorem in this talk.

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