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Research progress on mixed-integer nonlinear programming

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1 Introduction

The workpackage WP2 is dedicated to mixed integer nonlinear optimization problems. This is a large problem class, that may combine continuous and discrete variables, as well as linear and non-linear polynomial constraints, with a strong modeling power.

The objective is to investigate general solution methods based on the dual theories of moments and sums of squares of polynomials and design efficient algorithms leading to good approximate solutions for various applications within combinatorial optimization, finance and operations research, quantum information and energy networks. Finding good matrix factorizations (with as few factors as possible) is another class of combinatorial problems that can be attacked using this type of methods.

This involves an in-depth study of the general theory of polynomial optimization, as well as some of its specializations and extensions.Specifically, the variables in polynomial optimization may be constrained to take only binary values, as is the case for many graph problems and combinatorial optimization problems, or to take only integer values, or possibly a mix of continuous and integer values, as is the case for applications to energy network problems.

A far reaching generalization is the problem of moments where one optimizes over measures rather than just vector variables, a general setting which captures in particular applications to finance.
The workpackage is divided in 3 tasks:

Task 2.1 Combinatorial optimization for graph problems (led by NWO-I). This task involves research of the interplay between polynomial and combinatorial optimization. Indeed, most combinatorial optimization problems have polynomial optimization reformulations that inherit some structure from the original, like sparsity and symmetry. The polynomial optimization reformulations allow application of approximation hierarchies, like the Lasserre hierarchy, that are based on Positivstellensatz results from real algebraic geometry (or on the dual theory of moments). Non-commutative analogues of these hierarchies will be investigated in order to approximate hard optimization problems involving positive operator valued variables, arising in control and quantum information, like eigenvalue optimization and testing quantum graph isomorphism.

Task 2.2 Binary polynomial programming (led by UTIL). A famous example of binary polynomial programming is the quadratic assignment problem as first studied by the Nobel prize winners Koopmans and Kantorovich. These problems are NP-hard and notoriously hard to solve in practice. Different polynomial optimization formulations of such problems may lead to new computational approaches. As in Task 2.1, an important issue is to exploit the algebraic structure, mostly symmetry. Other important applications of binary polynomial optimization problems are in finance and operations research, for example in portfolio optimization.

Task 2.3 Mixed-integer optimization for network problems (led by Artelys). Optimization problems, which appear in network design, involve integer and continuous variables. An important issue is how to combine the exploration of discrete spaces with continuous non-linear optimization. We plan to develop new methods to integrate branch-and-bound methods and convex relaxations based on moment formulations, exploiting the properties of network optimization problems. Developing such algorithms for the efficient solutions of this class of problems is of particular interest from both theoretical and practical viewpoints.

2 Status of research performed by ESRs

The ESR's involved in this workpackage have worked on the above mentioned aspects. In particular, they have worked on combinatorial optimization problems like the maximum stable set problem (ESR7 and ESR8), on the optimal power flow problem (ESR15) and on matrix factorization problems (ESR6). More specifically, ESR7 is investigating several natural sum-of-squares based hierarchies for $\alpha(G)$ (the maximum stable set in G), with a focus on the open conjecture whether these hierarchies have finite convergence. ESR8 investigates a class of polynomial optimization problems over the simplex (including computing $\alpha(G)$) from the general perspective of the problem of moments, with a focus on analyzing the quality of the bounds in the hierarchy. ESR15 investigates the sum-of-squares hierarchies for optimal flow power problems, that involve both discrete/continuous variables and linear/quadratic constraints. He also investigates some dedicated heuristics for these problems. Finally, ESR6 investigates moment-based hierarchies for some matrix factorization problems, like finding the cp-rank of a matrix A, i.e., the smallest number of nonnegative rank 1 matrices summing up to A, and the separable rank of a matrix (related to the problem of testing entanglement in quantum information).

We refer to the following paragraphs where each ESR has presented some of his main results in some more details.

2.1 ESR6 - Andries Steenkamp/CWI

It is a common approach in mathematics to try to break complex objects into simpler parts. A familiar example is factorization of matrices. In general, a factorization of a matrix $A \in \mathbb{R}^{n\times m}$, over a family of cones $\{K_i\}_{i\in\mathbb{N}}$, each equipped with some inner product $\langle\cdot,\cdot\rangle$, is a collection of vectors $X_1,..,X_n,Y_1,..,Y_m \in K_r$ for some integer r, such that $A_{i,j} = \langle X_i, Y_j\rangle$ for all $(i,j)\in[n]\times[m]$. The least r for which one can factorize A in this way, is called the *rank* of A over the family of cones $\{K_i\}_{i\in\mathbb{N}}$. The factorization is said to be *symmetric* if $n = m$ and $X_i = Y_i$ for all $i \in [n]$.

Our research focuses on computing the cp-rank of a matrix (where we consider symmetric factorizations using the cones $K_i = \mathbb{R}^i_+$) and extending our results to the separable-rank. Computing the cp-rank of a matrix is of great practical and theoretical interest [BSM03]. The separable-rank is a parameter with applications in quantum information theory [CN20].

Recall that a symmetric nonnegative matrix, $0 \le A \in \mathcal{S}^n$, is said to be *completely positive*, if there exist $r-$many nonnegative vectors $a_1,...,a_r \in \mathbb{R}^n_+$ such that $A = \sum_{\ell=1}^r a_\ell a_\ell^T$. Suppose that r is the smallest integer for which this is possible, then r is called the *cp-rank* of A, denoted by $\mathrm{rank}_{\mathrm{cp}}(A)$. Computing the cp-rank, has been shown to be an NP-hard problem [Vav09]. Thus a need has arisen to find efficient methods for computing lower bounds. For the cp-rank, our research focuses on one such method coming from polynomial optimization, in particular the moment relaxation side [GLL19].

Start by setting $r := \mathrm{rank}_{\mathrm{cp}}(A)$ and fixing a a cp-factorization for A:

$$A = \sum_{\ell=1}^{r} a_\ell a_\ell^T, \text{ where } a_1,..,a_r \ge 0.$$

Then define, for each $\ell \in [r]$, the evaluation functional L_{a_ℓ} that maps a polynomial $p \in \mathbb{R}[x_1,x_2,...,x_n]$ to its evaluation $L_{a_\ell}(p) = p(a_\ell) \in \mathbb{R}$. Summing over ℓ we obtain the linear functional $L := \sum_{\ell=1}^r L_{a_\ell}$ from which we can recover the cp-rank by evaluating L at 1, i.e., $L(1) = \mathrm{rank}_{\mathrm{cp}}(A)$. This formulation of the cp-rank serves as a template for designing a hierarchy of semidefinite programs with solutions converging to a lower bound of $L(1)$. The quality of these bounds depends on which properties of L are imposed as constraints in the hierarchy. We are currently exploring the benefits of adding a constraint based on the following positivity property of L:

$$L(G_A) \succeq 0, \text{ where } G_A := A - [x_1,x_2,...,x_n][x_1,x_2,...,x_n]^T.$$

Namely, we impose the constraint:

$$M(G_A \otimes L) := L(G_A \otimes [\mathbf{x}][\mathbf{x}]^T) \succeq 0, \text{ where } [\mathbf{x}] \text{ is the monomial vector.}$$

In particular, we are running numerical experiments to see if, by using this additional constraint, one can improve upon previous lower bounds.

The above machinery can be extended to the separable rank, which can be defined as follows. For positive integers d_1, d_2, a matrix $\rho \in \mathbb{C}^{d_1 \times d_1} \otimes \mathbb{C}^{d_2 \times d_2}$ is said to be *separable* if there exists an integer r and vectors $a_\ell \in \mathbb{C}^{d_1}, b_\ell \in \mathbb{C}^{d_2}$ for $\ell \in \{1, 2, 3, ..., r\}$, such that

$$\rho = \sum_{\ell=1}^{r} a_\ell a_\ell^* \otimes b_\ell b_\ell^*.$$

Such ρ is then called *separable*, while positive semidefinite $\rho \in \mathbb{C}^{d_1 \times d_1} \otimes \mathbb{C}^{d_2 \times d_2}$ that do not admit such a decomposition are known to be *entangled* [CN20]. As before the smallest r for which this is possible is called the separable-rank of ρ. We have formulated a moment-based hierarchy of lower bounds for the separable rank, which also uses an analogue of the above positivity constraint. The next steps are getting a numerical implementation to test the quality of our lower bounds. We have already written up some of our results and work toward wrapping up a preprint.

The reported work contributes to Task 1.3, Workpackage 1 and Task 2.1.

2.2 ESR7 - Luis Felipe Vargas Beltran/CWI

Let $G = (V, E)$ be a graph. A subset of vertices $S \subseteq V$ is stable if there is no edge of G contained in S and the stability number of G, denoted by $\alpha(G)$ (or α if it is clear what is the graph) is the maximum size of a stable set in G. Computing the stability number is an NP-hard problem. However, it can be formulated as a polynomial optimization problem and then we can approximate the stability number with different techniques from the literature, such as via Lasserre hierarchy.
The starting point to define the hierarchies of approximation for the stability number is the Motzkin-Strauss formulation:

$$\frac{1}{\alpha(G)} = \min x^T (A_G + I) x \text{ subject to } x \geq 0, \sum_{i=1}^{n} x_i = 0. \tag{M-S}$$

Also, we can formulate the above problem (M-S) as an optimization problem over the sphere:

$$\frac{1}{\alpha(G)} = \min x^{\circ 2^T} (A_G + I) x^{\circ 2} \text{ subject to } x_1^2 + x_2^2 + \cdots + x_n^2 = 1, \tag{M-S-Sphere}$$

where $x^{\circ 2} = (x_1^2, \ldots, x_n^2)$. Hence, we can define the SOS-Lasserre hierarchies based on these two formulations. Let us define the polynomials $f_G(x) = x^T(I + A_G)x$ and $F_G(x) = f_G(x^{\circ 2}$. Then, let $f_G^{(r)}$ and $F_G^{(r)}$ denote, respectively, the order-r SOS-Lasserre bound based on the above simplex and sphere formulations.

Two other hierarchies for the stability number were introduced by de Klerk and Pasechnik [KP02]:

$$\zeta^{(r)}(G) = \min \left\{ \lambda : \lambda(A + I) - ee^T \in \mathcal{C}_n^r \right\},$$
$$\vartheta^{(r)}(G) = \min \left\{ \lambda : \lambda(A + I) - ee^T \in \mathcal{K}_n^r \right\}.$$

Here, the cones $\mathcal{C}_n^r$, $\mathcal{K}_n^r$ are subcones of the cone of copositive matrices defined by

$$\mathcal{C}_n^r = \Big\{ M \in \mathcal{S}^n : \Big(\sum_{i=1}^{n} x_i \Big)^r x^T M x \text{ has nonnegative coefficients} \Big\},$$

$$\mathcal{K}_n^r = \Big\{ M \in \mathcal{S}^n : \Big(\sum_{i=1}^{n} x_i^2 \Big)^r (x^{\circ 2})^T M x^{\circ 2} \text{ is a sum of squares} \Big\}.$$

In [KP02] the authors conjectured that $\vartheta^{(\alpha(G)-1)}(G) = \alpha(G)$ for any graph G. In fact, it is not even known if finite convergence holds for this hierarchy, that is, whether, for any graph G, there exists r for which $\vartheta^{(r)}(G) = \alpha(G)$. We have been working on this open problem.

We can prove the following relation between the hierarchies:

$$\alpha(G) \leq \vartheta^{(2r)}(G) = \frac{1}{F_G^{(2r+2)}} \leq f_G^{(r+1)} \text{ for all } r \in \mathbb{N}.$$

Hence, analyzing the finite convergence of the de Klerk-Pasechnik hierarchy $\vartheta^{(r)}(G)$ is equivalent to analyze the finite convergence of the Lasserre hierarchy based on the sphere formulation and weaker than the finite convergence of the Lasserre hierachy based on the simplex formulation. This observation allows us to prove finite convergence of the de Klerk-Pasechnik hierarchy for the class of *acritical graphs*, i.e., the graphs with no critical edges. Recall that an edge e is said to be *critical* if $\alpha(G - e) > \alpha(G)$. The key point for proving finite convergence of the Lasserre hierarchy is that for this case the problem has finitely many minimizers and then we can apply a result of Nie [Nie14] (based on Marshall's Bounded Hessian Condition).
Our approach now is to perturb the Motzkin-Straus formulation to force it to have finitely many minimizers. Namely, for any $\epsilon > 0$, we have:

$$\frac{1}{\alpha(G)} = \min x^T((1+\epsilon)A_G + I)x \text{ subject to } x \geq 0, \sum_{i=1}^{n} x_i = 0. \tag{M-S-ϵ}$$

Analogously, we can define the corresponding ϵ-hierarchies $\zeta_\epsilon^{(r)}(G), \vartheta_\epsilon^{(r)}(G), f_{G,\epsilon}^{(r)}$ and $F_{G,\epsilon}^{(r)}$, for which we have the relations:

$$\alpha(G) \leq \vartheta_\epsilon^{(2r)}(G) = \frac{1}{F_{G,\epsilon}^{(2r+2)}} \leq f_{G,\epsilon}^{(r+1)} \text{ for all } r \in \mathbb{N}.$$

The difference now is that, since the simplex (and the sphere) formulation has finitely many minimizers, we are able to prove finite convergence in general for the ϵ-pertubed hierarchies for any $\epsilon > 0$ and hence $\vartheta_\epsilon^{(r)}(G) = \alpha(G)$ for some $r \in \mathbb{N}$. Another property is that the linear de Klerk-Pasechnik bound is independent on ϵ, that is, $\zeta_\epsilon^{(r)}(G) = \zeta^{(r)}(G)$ for any $r \in \mathbb{N}$ and $\epsilon > 0$. One future goal is to understand the relation between the hierarchies $\vartheta_\epsilon^{(r)}$ and $\vartheta^{(r)}$, for which we can prove equality in the level $r = 0$. This raises the question, whether $\vartheta_\epsilon^{(r)}(G) = \vartheta^{(r)}(G)$ for all $r \in \mathbb{N}$. If this would be true then we would obtain finite convergence for *all* graphs. We are currently wrapping our results in the form of a preprint to be submitted

The reported work contributes to Task 2.1.

2.3 ESR8 - Felix Kirschner/UvT

As many of the problems that are to be addressed in WP2 are NP-hard in general it is interesting to study suitable approximation schemes. Of special interest is the convergence behavior of such approximation hierarchies, which often depends on the underlying feasibility set. Considering classical sets like the sphere $\mathbb{S}^n$, simplex Δ_n or the n-dimensional box $[-1,1]^n$ makes it easier to analyze said hierarchies. In our first project we analyzed RLT- and Lasserre-type approximation hierarchies for the generalized problem of moments over the simplex. We proved a convergence rate of $O(\frac{1}{r})$ for both hierarchies using a classical result by Powers and Reznick [PR01], which provides a certificate of nonnegativity for polynomials positive over the simplex. Our result is applicable to the stability number of a graph, which can be formulated as a quadratic polynomial optimization problem over the simplex Δ_n.

$$\frac{1}{\alpha(G)} = \min_{x \in \Delta_n} x^T(A+I)x,$$

where $G = (V, E)$ is the graph in question with $|V| = n$, A its adjacency matrix and I the identity matrix. We found that our linear hierarchy is in fact a generalization of a graph parameter introduced by De Klerk and Pasechnik [KP02], namely

$$\zeta^{(r)}(G) = \min \left\{ \lambda : \lambda(A+I) - ee^T \in \mathcal{C}_n^r \right\},$$

where e is the all-ones vector and $\mathcal{C}_n^r$ is an outer approximation of the cone of symmetric copositive matrices. One has $\alpha(G) \leq \zeta^{(r+1)}(G) \leq \zeta^{(r)}(G)$. Using a closed form expression of $\zeta^{(r)}(G)$ found by Pena,

Vera and Zuluaga [PVZ07] and some available results about this parameter we found our convergence rate of $O(\frac{1}{r})$ to be tight. Both hierarchies were implemented in Julia.
The MAX-CUT problem can be formulated as a quadratic polynomial optimization problem over the n-dimensional hypercube $[-1,1]^n$. The maximum cut of a graph G is equal to the optimal value of the following optimization problem.

$$\max_{x\in[-1,1]^n} x^T L x,$$

where L is the Laplacian matrix associated to G. Hence, insights about approximation hierarchies for quadratic polynomials over the hypercube are already of interest.
In our current project we are studying approximation kernels. Given a smooth function f defined on $[-1,1]^n$ the goal is to approximate f by a sequence of polynomials of increasing degree such that the sequence converges to f uniformly on $[-1,1]^n$. Formally, we consider the sequence of positive linear approximation operators:

$$\mathcal{K}^{(r)}(f)(x) = \int_{[-1,1]^n} f(y)K_r(x,y)d\mu(y),$$

where K_r is our approximation kernel and μ is a probability measure on $[-1,1]^n$. The kernels that qualify themselves as suitable for our task must fulfill certain properties. We aim to gain a deeper understanding of the *optimal* kernels, in the sense that they lead to the quickest uniform convergence. We emphasize that these kernels may also be utilized to bound the convergence rate of the Lasserre hierarchy of lower bounds over the hypercube under some assumptions.

The reported work contributes to Task 2.2.

2.4 ESR15 - Edgar Fuentes/Artelys

ESR has first focused on the application of Polynomial relaxations towards solving Optimal Power Flow (OPF) problems.

Such optimization problems in power systems, usually also comprise binary or integer decision variables related to the adjustment of equipments such as shunts or tap changers.
The integration of such equipments in the nonlinear OPF and its polynomial relaxation have been studied, as well as some heuristic scheme in order to create good integer solutions to the original problem. The heuristic created, combines rounding techniques, partial fixing, local search and relaxation of remaining binary decisions through complementarity constraints. First results obtained are quite promising and compares well versus existing schemes such as the *Tight and Cheap* relaxation [BAD19].

Future researches will improve this scheme and port it to distribution network problems, especially in order to find feasible solutions to existing problems where the nonlinear non convex approach often converges to infeasible points.

The reported work contributes to Task 2.3.

3 Related activities of the network in WP2

3.1 CWI

The group at CWI has been doing some work on related topics of mixed-integer programming. We just mention some recent work by Monique Laurent and Lucas Slot (PhD at CWI) on binary polynomial optimization problems. There the problem is to minimze a polynomial f over the boolean cube $\{0,1\}^n$. This problem is NP-hard as it permits, for instance, to model the max-cut problem and the problem of computing the stability number $\alpha(G)$ of a graph. In the recent preprint: *Sum-of-squares hierarchies for binary polynomial optimization* (arXiv:arXiv:2011.04027) we analyze the quality of the bounds obtained from the Lasserre hierarchy at order r, in the regime when r/n is constant. The main result is deriving an estimate for the error that relates to the extremal roots of the Krawtchouk polynomials. This work has been presented by Lucas Slot at the the Second POEMA Workshop on 20 October 2020.

3.2 UvT

On the topic of mixed-integer nonlinear programming, the group in Tilburg has also published some work and software where the ESR5 (Felix Kirchner) was not involved. This concerns the paper *Minimum energy configurations on a toric lattice as a quadratic assignment problem* by Daniel Brosch and Etienne de Klerk, to appear in *Discrete Optimization*. In addition the same authors have made a Julia software package available that performs pre-processing for semidefinite programming relaxations of comnbinatorial optimization problems, by doing a so-called Jordan symmetry reduction. This work will be presented in the POEMA 2nd Workshop on November 26, 2020 (online).

3.3 Artelys

Artelys offers optimization modeling, software and consulting services to clients about mathematical optimization. Therefore, the company is involved on numerous optimization projects using nonlinear mixed integer programming.

The most noticeable progress achieved this past year and not directly related to a client project are related to the nonlinear optimization solver *Artelys Knitro*. `Knitro` is a general purpose nonlinear optimization solver capable of handling structured (LP, QP, QCQP, SOCP) as well as blackbox nonlinear optimization problems. The solver has multiple algorithms embedded for nonlinear optimization as well as capability to address mixed integer nonlinear problems (MINLP) through the use of branch and bound or outer approximations.

This past year, we have been heavily working on the improvement of the solver towards solving MINLP. We recently introduced automated cuts generation for nonlinear optimization problems and root node branch and cut algorithm in order to make the best use of these cuts. Noticeably, the upcoming Knitro 12.3 release will include lift and project cuts derived from nonlinear equations (provided through callbacks). These strong cuts will therefore apply to any type of problem and allow solving more MINLP than before and faster.

The effort towards improving performances of Artelys Knitro for MINLP will still be ongoing in the foreseeable future, with the aim to offer a state of the art solver with best possible performances towards solving general mixed-integer nonlinear optimization problems.

4 Conclusion

The ESR's involved in this workpachage WP2 have achieved very good progress already. They have also identified several promising research questions left open at this stage and on which they will work in the near future. The future steps will include wrapping the results obtained so far in the form of preprints and submit them for publication, and pursue their research along the the promising open questions they have encountered. There is also a clear synergy between some the research directions, which is being deployed and exploited through the various events in the POEMA network and local activities at the various sites, at which the ESR's participate and give presentations.

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