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Research progress on exploiting structures in polynomial optimization

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1 Introduction

This document captures the first report on research progress within the area of exploiting structures in polynomial optimization. The objective of this workpackage is to exploit additional structures which appear in polynomial optimization problems in order to improve the performance of the Semidefinite Programming solvers and the numerical quality of their solution with a focus on the following points:

- Improvement of the performance of SDP relaxation methods by exploiting the underlying algebraic structure.
- Improvement of the numerical solution of SDP relaxation technique.
- Development of new relaxation methods, which exploit the structure of the nonlinear optimization problem.
- Improvement of existing SDP algorithms and software by exploiting the structure of various SDP relaxations.

Its is divided in the following tasks:

Task 3.1 Enhance performances by exploiting algebraic structures (led by Inria). The formulation of Nonlinear Global Optimization Problems in terms of moment problems and Semidefinite Programming relaxations inherits naturally from the algebraic structure of the optimization problem. Exploiting this algebraic structure is a critical issue to enhance the performance of relaxation methods in order to solve medium to large-scale global optimization problems. We plan to develop new methods, which can take into account the possible symmetries of a problem, or the sparsity of the moment formulation or directly the polynomial constraints involved in the nonlinear optimization problem to reduce the size of the SDP problems to be solved and to improve their convergence.

Task 3.2 Enhance numerical quality of solutions produced by optimization solvers (led by UiT). Solving of polynomial optimization problems relies on the computation of moments by Semidefinite Programming techniques, which are based on convex optimization in the cone of positive Hankel matrices associated to monomial bases. The aim of the task is to develop new methods that take into account this type of structure to improve the numerical quality of the SDP relaxation. We will work on the construction of bases adapted to the SDP problem, on the reconstruction of global optimizers from the solutions of SDP relaxation problems, on the quality of approximation of the global optimizers, on the certification of the results produced by numerical SDP solvers and on the robustness of the relaxation methods when the input polynomial constraints are known with some uncertainty.

Task 3.3 Algorithms and software for linear and nonlinear convex conic optimization (led by FAU). Existing SDP software, such as MOSEK and PENSDP, has been developed for general linear SDP problems. In the pre-processing phase, the software may try to recognize the structure of the problem and use it to more efficient solution. This may, however, be not always successful and sufficient. We will aim to develop special purpose algorithms and software, based on the existing ones that will expect the problem to be of special structure, such as rank-n data matrices or data matrices with certain sparsity structure. This should be utilized for substantial performance enhancement of the resulting software. Existing software is almost exclusively intended for linear SDP problems, although most of the codes rely on convergence theory for general nonlinear convex problems. We will further aim to develop efficient algorithms and software for general nonlinear convex SDP optimization, where the non-linearity can be either in the objective function, or in the matrix inequality constraints.

2 Status of research performed by ESRs

2.1 ESR9 - Lorenzo Baldi/Inria

The research topic of ESR9, Lorenzo Baldi, is "Structure of moment problems and applications to polynomial optimization". He began his research work by studying the basics of Polynomial Optimization and then the relevant results in related fields (representation theorems in real algebraic geometry, graded and border bases, duality of finitely generated algebras, conic duality, infinitely dimensional and truncated moment problem). The goal of Polynomial Optimization is to find the infimum (minimum) of a polynomial function on a basic semialgebraic set. Lasserre proposed hierarchies of approximations for this problem. The ESR focused on the Moment approximation, which has better properties than the Polynomial one. In particular, the following questions were investigated:

- Do the Polynomial and Moment hierarchy have finite convergence to the minimum?
- Are the (truncated) moment minimizer sequences coming from measures ?

The ESR and his advisor gave positive answers to these questions for finite semialgebraic sets (under a small technical condition), and generic negative answer for semialgebraic sets of dimension ≥ 3.

Other questions that were investigated, related to Lasserre hierarchies, are the following:

- Can one compute also the minimizers, or equation for (the Zariski closure of) the semialgebraic set of minimizers, from the (truncated) moments?
- Can one modify any problem to have exactness (finite convergence + moments from measures)?

The answer to the first question is again positive for finite semialgebraic sets and in some good cases: in these cases the kernel of the Hankel matrix associated to a generic moment sequence gives generators for the (real) ideal defining the Zariski closure of the semialgebraic set. For the second answer some problems concerning the description of singular points in the non equidimensional case (when we cannot use the Jacobian rank conditions) arose, because localizing to irreducible components is very inefficient from a computational point of view. Results in specific cases (isolated singularities in an equidimensional semialgebraic set) were obtained. The approach is based on a generalization of the KKT conditions (and thus of the Gradient Ideal). Finally, the ESR started implementing and testing the results in a Julia package MomentTools.jl,and is writing an article containing the results ("Exact Moment Representation in Polynomial Optimization").

The reported work contributes to Task 3.1.

2.2 ESR10 - Tobias Metzlaff/Inria

The research topic of ESR10, Tobias Metzlaff, is "Group theoretic Polynomial Bases for Global Optimization". The ESR and his supervisor started with the idea of using the common zeros of multivariate Chebyshev polynomials as nodes for a Gaussian cubature formula. A cubature of degree d is a linear form $\Lambda \in \mathbb{K}[X]^*$, that satisfies $\Lambda(f) = \mathcal{I}(f)$ for all polynomials f with degree $\leq d$, where $\mathcal{I}$ is an integration operator defined by a weight function. When Λ is defined as a weighted sum of evaluations at fixed nodes, then the cubature is called Gaussian, if it attains the minimal number of nodes. In the beginning, the ESR studied classical univariate quadrature formulae, characterization of Gaussian cubatures, symmetry adaptation, moment methods, discrete Fourier analysis and interpolation theory.A concept of representation theory, that was used in the past years by several authors for discrete approximation, is the one of root systems. Root systems yield weight vectors and a fundamental domain, which is a compact, convex set with a "nice" shape (equilateral triangle, tetrahedron, ...). Considering the orbit of this domain under the action of the reflection group associated to the root system, one can formulate invariance constraints. This introduces spaces of invariant and anti-invariant functions with elementary generators, that correspond to the fundamental weight vectors of the root system. Similar to the univariate case, one can then define generalized Chebyshev polynomials. A geometric relation between the fundamental domain and the periodicity domain of the weight lattice was formalized and proven. The Chebyshev polynomials are maps on a deformed domain with cusps, which is the image of the fundamental domain under the elementary group-invariant functions. A remarkable property of these polynomials is, that they form an orthogonal polynomial basis on this deformed domain with respect to a certain weight function. A proof is ensured by the above mentioned geometric relation. With this setup the common zeros of the Chebyshev polynomials were investigated. It was discovered, that their number is maximal and they coincide with points in a down-scaling of the weight lattice, an indication for nodes of a Gaussian cubature. However, this only holds for certain types of root systems. For the other types, one can construct near-minimal formulae or use Chebyshev polynomials of the second kind for two variables. The necessary procedures to analyze geometric properties were programmed in Maple and the current work is the extension of these results to the case of arbitrary number of variables and on better understanding the concept of Lebesgue constants to measure the error of a cubature formula in the operator norm. Next to his own research, the ESR also participated in the events organized by the POEMA network and attended other conferences or seminars related to his work.

The reported work contributes to Task 3.2.

2.3 ESR11 - Sebastian Debus/UiT

The research topic of ESR 11, Sebastian Debus research, concerns applications of invariant theoretical methods within real algebra in particular with respect to polynomial optimization and quadrature rules. The overreaching goal of his project is to understand the effects that group actions have on specific problems and to exploit these effects to gain computational efficiency and numerical accuracy. The focus of his research during the first year have been finite reflection groups, and in particular their invariant theory and their representation theory. In this context he submitted together with his supervisor Cordian Riener a paper which studies in detail the question of non-negativity of forms invariant under reflection groups of type $A_{n-1}, B_n, D_n, I_2(k)$. In particular, the results obtained in this paper allow for a better understanding of the difference between non-negative polynomials and sums of squares in equivariant situations. Furthermore, a enhanced discussions with ESR 3, Markus Breivik, during the virtual secondment at Uni Konstanz initiated a research project on topological complexity of semi-algebraic sets. Using symmetry reduction techniques, it might be able to improve bounds on Betti numbers for projections of semi-algebraic sets. Such bounds can be seen as indicators of computational complexity of certain algorithmic tasks, for example, quantifier elimination, which is a fundamental task in real algebraic geometry.

The reported work contributes to Task 3.1 and Task 3.2.

2.4 ESR12 - Arefeh Kavand/FAU

The topic of ESR12, Arefeh Kavand, is the development of *algorithms and software for nonlinear convex conic optimization*. In the first months of the project the ESR has been exploring the concept of generalized Augmented Lagrangians for the solution of semidefinite programs. This has been done with a particular focus on structures and difficulties which arise in the polynomial optimization context. The main two aspects which have been taken into account so far are the ill-conditioning and a low rank structure in the data.

In order to face the problem of ill-conditioning was approached, a general class of barrier functions (so called penalty-barrier-functions) was suggested, which provides an upper bound for the eigenvalues of the Hessian of the Augmented Lagrangian. While such an approach has been reported in literature before, in our project, we combine it with a regularization technique, which provides - in addition - a uniform lower bound for the Eigenvalues.

Another important aspect is that - when applying penalty-barrier-functions in the context of semidefinite programming - the computational complexity for assembling the Hessian matrix is one order of magnitude higher than in comparable approaches using modified barrier functions or even the well known $\log\det$-function as used in interior point methods. In our project, we were able to show that, when combining the Penalty-Barrier-Concept with iterative solutions methods for the solution of arising Newton-type systems, this disadvantage can be fully eliminated. This is of particular interest for polynomial optimization problems, as for tight approximations, often very large SDPs are obtained. In this cases assembling the full Hessian of the Augmented Lagrangian is expensive and sometimes the Hessian can not even be stored.

A third part of the work of ESR12 during the first months was that for the first time so called primal-dual Penalty-Barrier-Multiplier methods for semidefinite programming could be developed (PD-PBM). A basic layout of the algorithm has been designed and a prototypical implementation in Matlab is available. One of the major goals will now be to prove in theory and practise that this new class of algorithms has advantages in general (e.g. a faster rate of convergence is expected compared to purely primal methods), and in particular, when applied to certain types of polynomial optimization problems. One thing, which has been already observed is that the primal-dual approach helps to circumvent problems with ill-conditioning which - despite the measures described above - can, depending on the particular problem data, not be entirely eliminated in the purely primal solution process.

In addition to these activities, ESR12 has been cooperating with ESR13 to work on preconditioners helping to cope with the high computational complexity expected for large polynomial optimization problems provided by our partners in future.

Currently, we are writing our first joint paper with UoB with the tentative title "Penalty methods for low-rank semidefinite programming with application to truss topology optimization".

The reported work contributes to Task 3.3.

2.5 ESR13 - Soodeh Habibi/UoB

The topic of ESR13, Soodeh Habibi, is the development of *algorithms and software for structured semidefinite optimization*. The goal is to solve large-and-sparse low-rank semidefinite programs (SDP) by using a variant of an interior point method. Interior-point methods are kind of a techniques to convert the conic problems into a sequence of unconstrained problems. The bottleneck in an interior-point method consists in assembling and solving the so-called Schur complement equation, a large system of linear equations with a positive definite matrix. As the matrix is large and sparse, the Schur complement equation can be solved by using an Krylov type iterative method such as the conjugate gradient (CG) method. The convergence rate of such a method is usually slow due to ill-conditioning of the matrix. In fact, the Schur complement matrix becomes increasingly ill-conditioned as the interior-point method makes progress towards the solution. Hence, to solve the linear system, instead of CG we are using a modified version of that which is called Preconditioned Conjugate Gradient (PCG). Efficient preconditioners allow PCG to converge to a solution of the linear equation in a few iterations, independent of the ill-conditioning of the Hessian matrix.

Development of efficient preconditioners is very much problem dependent. In our research, we are focusing on SDP problems with (expected) very low rank of the solution matrix. Using this and further assumption we have proposed two new preconditioners, inspired by the article Richard Y. Zhang and Javad Lavaei, "Modified Interior-Point Method for Large-and-Sparse Low-Rank Semidefinite Programs". Numerical experience shows that our modified preconditioners are more efficient than those by Zhang and Lavaei. Moreover, our interior-point method with the new preconditioners is substantially faster than standard available software for SDP, such as MOSEK. Our main focus is on solving large-scale problems resulting from truss topology optimization. Currently, we are writing our first joint paper with FAU under the title of "Penalty methods for low-rank semidefinite programming with application to truss topology optimization".

The reported work contributes to Task 3.3.

3 Related activities of the network in WP3

3.1 Inria

We started investigating the structure of Polynomial and Moment Optimisation problems, in two directions.

The first one aims at exploiting symmetries in moment problems, in order to improve the efficiency of their solutions. A first step in this direction is to find symmetry adapted representation and good basis for invariants and covariants. The special case of finite groups and in particular reflexion groups is considered. Work on root systems and generalized multivariate Chebyshev polynomials have been developed in the quest of good bases for symmetry adapted representations.

Experimentation with the Computer Algebra system Maple have been developed to evaluate the performance of the approach. The next step will consist in connecting this representation with symmetric moment optimization problems.

The second direction of investigation focuses on analyzing the structure of cones of moments, involved in the Sum of Squares (SoS) and Moment Matrix (MoM) convex relaxations of polynomial optimization problems. We develop and analyze in details the notion of exact MoM relaxations, where moment minimizer sequences are coming from measures. In this ideal situation, the minimum of the polynomial problem, as well as all the minimizer points, can be recovered from the moment sequence.

New conditions for MoM exactness have been obtained, including optimisation on finite semi-algebraic sets, finite set of minimizers, Boundary Hessian Conditions. A package MomentTools, in the language Julia, has been developed to validate experimentally and in particular numerically the properties that are analyzed. An article on these results is in progress and should be submitted soon for publication in a journal.

3.2 UiT

A main focus of the research activities done at UiT in the context of WP3 are concerned with symmetries in polynomial optimization. Together with ESR 11 we are working on a better understanding of the effects of group actions on polynomial optimization problems. In a first step we were focusing on a deeper understanding of the difference between sums of squares and non-negative polynomials, in the case of invariant polynomials. Using a combination of invariant theory and representation theory we were able to provide novel characterisations in the context of polynomials which are invariant by finite reflection groups. Furthermore, during the secondment of ESR11 at University of Konstanz a collaboration between ESR11 and ESR3 (Markus Breivik) was initiated. Finally, we are working on a better understanding on the so called Specht polynomials and their varieties in the context of finite reflection group. It is our hope that this enhanced understanding will allow for new generalizations of results used to exploit symmetries in the context of symmetric polynomials to more general classed of groups.

3.3 FAU & UoB

The research teams at FAU and UoB have close scientific interaction on the research work in this workpackage. In the summer term they have started to organize meetings between UoB and FAU on a regular basis (approximately biweekly). In these meetings ideas between ESR12 and ES13 (and their advisors) on the development of optimization solvers taking structures specific to polynomial optimization problems into account are exchanged. This includes a common data and software basis, maintained by the two groups. A particular focus of these meetings so far was to identify common structures in interior point methods and primal-dual methods based on Augmented Lagrangians. It turned out that the linear systems which have to be solved at the core of both methods have a mathematically equivalent structure. Thus it seems possible to develop iterative methods and, in particular, preconditioners, which can be applied in the framework of both solution concepts. These methods have been tested by means of problems from truss topoplogy design. Their scope will be extended to more general polynomial optimization problems in the future.

4 Conclusions

In order to improve the computational possibilities as well as the numerical stability of semidefinite programming as well as semidefinite relaxations it is of vital importance to take specific characteristics of the problems into considerations. The research results which have already been obtained and will be obtained within this work package will play a fundamental role here. As was presented in this report, all ESRs are actively contributing to these important questions and have, in particular, been able to advance on their individual projects. Although the global pandemic had certain effects also on the possibility of exchange between the nodes, we have been able to use virtual secondments as a way for additional exchange between the ESRs, which had further positive effects on the research work in WP3.

We expect that all of the ESRs will further their ongoing projects successfully in the coming year and also it can be expected that the global situation allows for more in person exchange again. This could also facilitate further collaborative exchange within the work package and among the ESRs.

Overall, we can conclude that WP3 is on track to deliver the research outcomes necessary to improve the performance of semidefinite programming and enhance the numerical stability of their solvers. Furthermore, we do not see any delay on the work of the individual ESRs, which are all well on track on the PhD projects.