

Designing and Implementing Algorithms for Mixed-Integer Nonlinear Optimization

Edited by

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Abstract

Mathematical models for optimal decisions often require both nonlinear and discrete components. These mixed-integer nonlinear programs (MINLP) may be used to optimize the energy use of large industrial plants, integrate renewable sources into energy networks, design biological and biomedical systems, and address numerous other applications of societal importance. The first MINLP algorithms and software were designed by application engineers. While these efforts initially proved useful, scientists, engineers, and practitioners have realized that a transformational shift in technology will be required for MINLP to achieve its full potential. MINLP has transitioned to a forefront position in computer science, with researchers actively developing MINLP theory, algorithms, and implementations. Even with their concerted effort, algorithms and available software are often unable to solve practically-sized instances of these important models. Current obstacles include characterizing the computability boundary, effectively exploiting known optimization technologies for specialized classes of MINLP, and effectively using logical formulas holistically throughout algorithms.

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Edited in cooperation with Radu Baltean-Lugojan

1 Executive Summary

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This workshop aimed to address this mismatch between natural optimization models for important scientific problems and practical optimization solvers for their solution. By bringing together experts in both theory and implementation, this workshop energized efforts making MINLP as ubiquitous a paradigm for both modeling and solving important decision problems



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as mixed-integer linear programming (MIP) and nonlinear programming (NLP) have become in recent years. In particular, we highlighted:

- **MINLP Solver Software** Early in the workshop, the main developers of MINLP software packages outlined the current state of their software. This served as a needs analysis for the community to identify crucial areas for future development. We also dedicated a break-out session discussing best practices for conducting scientifically-meaningful computational experiments in MINLP.
- **Intersecting Mixed-Integer & Nonlinear Programming** MINLP is a superset of both mixed integer linear optimization and nonlinear optimization, so we leveraged the best methods from both by incorporating both sets of experts.
- **Driving Applications** Applications experts, e.g. in petrochemicals, manufacturing, and gas networks, offered their perspectives on what practitioners need from MINLP solvers. We dedicated an entire break-out session to energy applications and explored what are the needs for MINLP within the energy domain. During the open problem session, several other applications experts outlined other open problems in engineering.
- **Connections between MINLP and machine learning** Many machine learning challenges can be formulated as MINLP. Also, machine learning can significantly improve MINLP solver software. We explored these connections at length in a break-out session.

This seminar brought together an assortment of computer scientists with expertise in mathematical optimization. Many of the presentations were more theoretical and suggested new technologies that the solver software could incorporate. Other presentations were more practical and discussed building solver software or applying that software to specific domain applications.

As a result of this seminar, we are planning a special issue in the journal “Optimization & Engineering”. We are also working to turn the notes from our open problem session into a larger document that will start a conversation with the entire mathematical optimisation community. Participants broadly expressed that this week at Dagstuhl helped them workshop their papers, so several academic papers will explicitly mention the Dagstuhl seminar. Finally, a new set of metrics for comparing MINLP solvers were developed at this meeting and will greatly aid future solver testing.

2 Table of Contents

Executive Summary

Pierre Bonami, Ambros M. Gleixner, Jeff Linderoth and Ruth Misener 64

Overview of Talks

A deterministic global optimisation algorithm for mixed-integer nonlinear bilevel programs <i>Claire Adjiman</i>	69
Strengthened Semidefinite Relaxations for Quadratic Optimization with Switching Variables <i>Kurt M. Anstreicher</i>	69
Online generation via offline selection of strong linear cuts from QP SDP relaxation <i>Radu Baltean-Lugojan and Ruth Misener</i>	69
Finding feasible solutions in MINLP problems <i>Pietro Belotti</i>	70
Incorporating Quadratic Approximations in the Outer-Approximation Method for Convex MINLP <i>David Bernal Neira and Ignacio Grossmann</i>	70
Numerical Challenges in MINLP solvers <i>Timo Berthold</i>	71
Optimization using both models and input-output data <i>Fani Boukouvala</i>	71
SMT-based mixed non-linear optimization <i>Andrea Callia D’Iddio</i>	72
On some hard quadratic unconstrained boolean optimization problems <i>Sanjeeb Dash</i>	72
Subset selection with sparse matrices <i>Alberto Del Pia, Santanu Dey, and Robert Weismantel</i>	73
Robust Treatment of Non-Convex Optimization Problems with Application to Gas Networks <i>Denis Aßmann (FAU), Frauke Liers (FAU), Juan Vera (Tilburg), and Michael Stingl (FAU)</i>	73
New SOCP relaxation and branching rule for bipartite bilinear programs <i>Santanu Dey</i>	74
Deep Learning and Mixed Integer Optimization <i>Matteo Fischetti</i>	74
Improved quadratic cuts for convex mixed-integer nonlinear programs <i>Ignacio Grossmann</i>	75
Binary Extended Formulations for Mixed-Integer Linear Programs <i>Oktay Gunluk, Sanjeeb Dash, and Robert Hildebrand</i>	75
Disjunctive cuts and extended formulations for bilinear functions <i>Akshay Gupta</i>	76

Semidefinite Programming Cuts in Gravity <i>Hassan Hijazi</i>	76
Stronger polyhedral relaxations for polynomial optimization problems <i>Aida Khajavirad and Alberto Del Pia</i>	77
Mixed-Integer Nonlinear Programming Applications: Pyomo Tools for Tailored Strategies <i>Carl Damon Laird</i>	77
Global solutions of MIQCPs <i>Amélie Lambert</i>	77
Virtuous smoothing and more virtuous smoothing <i>Jon Lee, Daphne Skipper, and Luze Xu</i>	78
Mixed-Integer Derivative-Free Optimization <i>Sven Leyffer</i>	78
LP and SDP for kissing numbers <i>Leo Liberti</i>	79
External Intersection Cuts <i>James Luedtke and Eli Towle</i>	79
Automatic reformulations of convex MINLPs in Minotaur <i>Ashutosh Mahajan</i>	79
Optimising with Gradient-Boosted Trees and Risk Control <i>Miten Mistry, Dimitrios Letsios, Gerhard Krennrich, Ruth Misener, and Robert M. Lee</i>	80
Using 2D Projections for Separation and Propagation of Bilinear Terms <i>Benjamin Müller, Ambros M. Gleixner, and Felipe Serrano</i>	80
CIA Decomposition <i>Sebastian Sager</i>	80
ALAMO: Machine learning from data and first principles <i>Nikolaos V. Sahinidis</i>	81
Separating over the convex hull of MINL constraints <i>Felipe Serrano</i>	81
Product convexification: A new relaxation framework for nonconvex programs <i>Mohit Tawarmalani</i>	82
Mixed-integer convex representability <i>Juan Pablo Vielma</i>	82
Experimentation with MINLP solver software <i>Stefan Vigerske and Ambros M. Gleixner</i>	83
Integer Optimal Solutions are Sparse <i>Robert Weismantel</i>	83
Combining ADAL with Factorizing the Dual to Solve SDP <i>Angelika Wiegele</i>	83
Mixed-integer conic optimization and MOSEK <i>Sven Wiese</i>	84

Working groups

Applications in Energy	84
Sound experimentation with MINLP software	84
Connections between MINLP and Machine Learning	85
Open problems	
Mathematical Foundations	86
Computing Implications	86
Engineering Applications	86
Participants	87

3 Overview of Talks

3.1 A deterministic global optimisation algorithm for mixed-integer nonlinear bilevel programs

Claire Adjiman (Imperial College London, GB)

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Joint work of Claire Adjiman, Remigijus Paulavicius, Polyxenia-M. Kleniati
Main reference Polyxeni-Margarita Kleniati, Claire S. Adjiman: “A generalization of the Branch-and-Sandwich algorithm: From continuous to mixed-integer nonlinear bilevel problems”, *Computers & Chemical Engineering*, Vol. 72, pp. 373–386, 2015.
URL <http://dx.doi.org/10.1016/j.compchemeng.2014.06.004>

We present Branch-and-Sandwich, an algorithm for the global solution of mixed-integer nonlinear bilevel programs, based on a branch-and-bound framework in which branching is permitted on outer and inner variables. We discuss the tree management and bounding strategies, present some examples and introduce ongoing implementation efforts and a test library.

3.2 Strengthened Semidefinite Relaxations for Quadratic Optimization with Switching Variables

Kurt M. Anstreicher (University of Iowa, US)

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We consider indefinite quadratic optimization problems that include continuous and discrete variables of the form $F = \{(x, y) \mid 0 \leq x \leq y, y \in \{0, 1\}^n\}$. The binary y variables are often referred to as “switching” or “indicator” variables and occur frequently in applications. Our focus is to represent, or approximate, the convex hull of $\{(x, xx', y) \mid (x, y) \in F\}$ using constraints that include semidefiniteness conditions. We obtain an exact convex hull representation for $n = 2$ that also provides valid constraints that can be used to tighten semidefinite relaxations for higher n .

3.3 Online generation via offline selection of strong linear cuts from QP SDP relaxation

Radu Baltean-Lugojan (Imperial College London, GB) and Ruth Misener (Imperial College London, GB)

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Joint work of Radu Baltean-Lugojan, Ruth Misener, Pierre Bonami, Andrea Tramontani

Convex and in particular semidefinite relaxations (SDP) for non-convex continuous quadratic optimization can provide tighter bounds than traditional linear relaxations. However, using SDP relaxations directly in Branch&Cut is impeded by lack of warm starting and inefficiency when combined with other cut classes, i.e. the reformulation-linearization technique. We present a general framework based on machine learning for a strong linear outer-approximation

that can retain most tightness of such SDP relaxations, in the form of few strong low dimensional linear cuts selected offline. The cut selection complexity is taken offline by using a neural network estimator (trained before installing solver software) as a selection device for the strongest cuts.

3.4 Finding feasible solutions in MINLP problems

Pietro Belotti (Fair Isaac, GB)

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Finding feasible solutions in MINLPs is helpful beyond providing a sensible result to the solve process. In MINLP, especially the nonconvex variant, a good cutoff is of double usefulness in finding a global optimum as it reduces the tree search but also, most importantly, reduces variables bounds, which in turn results in a better linearization and hence a tighter lower bound.

We present two heuristics for MINLP: one is an ancient MINLP heuristic implemented in the very first version of Couenne, which is a probing-based rounding algorithm. The second is a heuristic to find a solution to a NLP problem that is currently used in the Xpress-SLP solver.

3.5 Incorporating Quadratic Approximations in the Outer-Approximation Method for Convex MINLP

David Bernal Neira (Carnegie Mellon University – Pittsburgh, US) and Ignacio Grossmann (Carnegie Mellon University – Pittsburgh, US)

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Joint work of David Bernal Neira, Ignacio E. Grossmann, Lijie Su, Lixin Tang, Jan Kronqvist

Main reference Lijie Su, Lixin Tang, David E. Bernal, Ignacio E. Grossmann: “Improved quadratic cuts for convex mixed-integer nonlinear programs”, *Computers & Chemical Engineering*, Vol. 109, pp. 77–95, 2018.

URL <http://dx.doi.org/10.1016/j.compchemeng.2017.10.011>

We present two new methods for solving convex mixed-integer nonlinear programming problems based on the outer approximation method. The first method is inspired by the level method and uses a regularization technique to reduce the step size when choosing new integer combinations. The second method combines ideas from both the level method and the sequential quadratic programming technique and uses a second order approximation of the Lagrangian when choosing the new integer combinations. The main idea behind the methods is to choose the integer combination more carefully in each iteration, in order to obtain the optimal solution in fewer iterations compared to the original outer-approximation method. We prove rigorously that both methods will find and verify the optimal solution in a finite number of iterations. Furthermore, we present a numerical comparison of the methods based on 109 test problems, which illustrates the benefits of the proposed methods.

3.6 Numerical Challenges in MINLP solvers

Timo Berthold (FICO – Berlin, DE)

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While numerics are already challenging us in MILP, it is my impression that in MINLP it is even more demanding to build a robust model and to develop a numerically stable solver. In MILP and MINLP solvers, reproducibility and reliability are key features to success. All major MILP solvers are deterministic, even in parallel mode, numerical tolerances are carefully chosen and various procedures and safety measures are implemented aiming for avoiding numerical issues, e.g. in presolving or cutting plane generation. In LP and MILP, there are approaches to solve problems to “true”, exact optimality. One possibility to extend those is the use of hybrid approaches like iterative refinement for LP and QP ([1]) or a hierarchy of dual bounding procedures for MILP ([2]). Then, in MILP models, challenges occur that are not present in MINLP, like super-linear error propagation, boundary conditions, and singular points. Moreover, some of the most-used solution methods are particularly prone to getting solutions which are “slightly off”. Take outer approximation as an example. Since we are approximating from the outside by cutting, we typically stop when the approximate solution is within the feasibility tolerances for the constraints, or differently speaking, violating them by the maximal amount that we are willing to tolerate. Also, vanishing eigenvectors are a problem in MINLP/OA which does not have a pendant in MILP.

I would like to kick off a discussion on:

- How are MINLP models different from MILP models?
- How can we measure the numerical conditioning of a MINLP model?
- Why are some of our standard solution approaches asking for numerical troubles and how can we address this?
- What would be an “exact” standard to compare floating-point, numerical-tolerance solvers against?
- Is numerical robustness a blocker for MINLP becoming an out-of-the-box tool like MILP?

References

- 1 Gleixner, Ambros M., Daniel E. Steffy, and Kati Wolter. “Iterative refinement for linear programming.” *INFORMS Journal on Computing* 28.3 (2016): 449–464.
- 2 Cook, William, et al. “A hybrid branch-and-bound approach for exact rational mixed-integer programming.” *Mathematical Programming Computation* 5.3 (2013): 305–344.

3.7 Optimization using both models and input-output data

Fani Boukouvala (Georgia Institute of Technology – Atlanta, US)

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Joint work of Fani Boukouvala, Jianyuan Zhai, Sun Hye Kim

In many engineering fields, there is a continuously increasing interest in coupling equation-based first-principle modeling with information that comes in the form of input-output data, in order to be able to optimize systems incorporating very detailed information regarding the material, flow, geometry, physical properties and chemistry of the systems. This need has given rise in developments of optimization methods that can optimize systems without

equations or derivatives, but simply with the exchange of input-output data streams. The typical applications of data-driven optimization, consider the system that needs to be optimized entirely as a “black-box”, however, many applications exist (i.e., process synthesis and design of modular manufacturing systems) which can be formulated as hybrid mixed integer nonlinear optimization problems, comprised of both explicitly known equations and black-box, or data-dependent equations. This talk highlights the need for MINLP solvers to be able to incorporate black-box components, and proposes ways of enabling this capability. Specifically, we propose several ideas for developing adaptive, flexible and tractable surrogate parametric functions to represent the input-output data and show their effectiveness in optimizing a library of benchmark problems, which are treated as black-box functions. In order to develop efficient and useful surrogate models, we borrow ideas from machine learning (i.e., feature selection), numerical integration (i.e., sparse grid sampling and polynomial interpolation) and optimization under uncertainty.

3.8 SMT-based mixed non-linear optimization

Andrea Callia D’Iddio (Imperial College London, GB)

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I would like to introduce ManyOpt, an optimization tool based on Satisfiability Modulo Theories (SMT). SMT solving can provide methods for feasibility checking whose main benefits are incrementality and deductive reasoning. Thanks to these benefits, it is possible to have a “warm start” in which an initial optimization problem is solved, and to take advantage of the learned information to solve extensions or modifications of that problem. This would be especially useful for what-if scenarios and for an interactive use of the tool. Experimental results with benchmarks from the MINLPLIB2 library show the effectiveness of the approach.

3.9 On some hard quadratic unconstrained boolean optimization problems

Sanjeeb Dash (IBM TJ Watson Research Center – Yorktown Heights, US)

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In this talk we discuss the solution of hard quadratic unconstrained optimization problems arising from Ising model problems defined on Chimera graphs.

3.10 Subset selection with sparse matrices

Alberto Del Pia (University of Wisconsin – Madison, US), Santanu Dey (Georgia Institute of Technology – Atlanta, US), and Robert Weismantel (ETH Zürich, CH)

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In subset selection we search for the best linear predictor that involves a small subset of variables. Due to the vast applicability of this model, many approaches have been proposed by different communities, including enumeration, greedy algorithms, branch and bound, and convex relaxations. Our point of departure is to understand the problem from a computational complexity viewpoint. Using mainly tools from discrete geometry, we show that the problem can be solved in polynomial time if the associated data matrix is obtained by adding a fixed number of columns to a block diagonal matrix. This is joint work with Santanu S. Dey and Robert Weismantel.

3.11 Robust Treatment of Non-Convex Optimization Problems with Application to Gas Networks

Denis Aßmann (FAU), Frauke Liers (FAU), Juan Vera (Tilburg), and Michael Stingl (FAU)

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Main reference D. Aßmann, F. Liers, M. Stingl, J. Vera: “Deciding Robust Feasibility and Infeasibility Using a Set Containment Approach: An Application to Stationary Passive Gas Network Operation”, 2017
URL <https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/136>
Main reference D. Aßmann, F. Liers, M. Stingl: “Decomposable Robust Two-Stage Optimization: An Application to Gas Network Operations Under Uncertainty”, 2017
URL <https://opus4.kobv.de/opus4-trr154/frontdoor/index/index/docId/209>

In this talk, we will study uncertain stationary gas network problems. We will first explain the concept that can also be applied in other contexts and will then make it concrete for the application. For passive networks, the task of deciding robust feasibility of the corresponding nonlinear two-stage fully adjustable problem is equivalent to deciding set containment of a projection of the feasible region and the uncertainty set. For answering this question, two polynomial optimization problems – one for showing feasibility and one for showing infeasibility – are developed.

For the case of networks with active elements such as compressors, we reformulate the robust two-stage problem and then apply a piecewise linear relaxation of the non-convex functions. It is shown that comparably large realistic instances can be solved in practice, with only a mild increase in conservatism due to the used piecewise linear relaxation.

This is joint work with Denis Aßmann, Michael Stingl (both FAU), and Juan Vera (Tilburg).

3.12 New SOCP relaxation and branching rule for bipartite bilinear programs

Santanu Dey (Georgia Institute of Technology – Atlanta, US)

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Joint work of Santanu Dey, Asteroide Santana, Yang Wang

A bipartite bilinear program (BBP) is a quadratically constrained quadratic optimization problem where the variables can be partitioned into two sets such that fixing the variables in any one of the sets results in a linear program. We propose a new second order cone representable (SOCP) relaxation for BBP, which we show is stronger than the standard SDP relaxation intersected with the boolean quadratic polytope. We then propose a new branching rule inspired by the construction of the SOCP relaxation. We describe a new application of BBP called as the finite element model updating problem, which is a fundamental problem in structural engineering. Our computational experiments on this problem class show that the new branching rule together with an polyhedral outer approximation of the SOCP relaxation outperforms a state-of-the-art commercial global solver in obtaining dual bounds.

3.13 Deep Learning and Mixed Integer Optimization

Matteo Fischetti (University of Padova, IT)

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Joint work of Matteo Fischetti, Jason Jo

Main reference Matteo Fischetti, Jason Jo: “Deep Neural Networks as 0-1 Mixed Integer Linear Programs: A Feasibility Study”, CoRR, Vol. abs/1712.06174, 2017.

URL <http://arxiv.org/abs/1712.06174>

Deep Neural Networks (DNNs) are very popular these days, and are the subject of a very intense investigation. A DNN is made up of layers of internal units (or neurons), each of which computes an affine combination of the output of the units in the previous layer, applies a nonlinear operator, and outputs the corresponding value (also known as activation). A commonly-used nonlinear operator is the so-called rectified linear unit (ReLU), whose output is just the maximum between its input value and zero. In this (and other similar cases like max pooling, where the max operation involves more than one input value), *for fixed parameters* one can model the DNN as a 0-1 Mixed Integer Linear Program (0-1 MILP) where the continuous variables correspond to the output values of each unit, and a binary variable is associated with each ReLU to model its yes/no nature. In this talk we discuss the peculiarity of this kind of 0-1 MILP models, and describe an effective bound-tightening technique intended to ease its solution. We also present possible applications of the 0-1 MILP model arising in feature visualization and in the construction of adversarial examples. Computational results are reported, aimed at investigating (on small DNNs) the computational performance of a state-of-the-art MILP solver when applied to a known test case, namely, hand-written digit recognition.

3.14 Improved quadratic cuts for convex mixed-integer nonlinear programs

Ignacio Grossmann (Carnegie Mellon University – Pittsburgh, US)

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Joint work of Ignacio Grossmann, Lijie Su, Lixin Tang, David E. Bernal

Main reference Marco A. Duran, Ignacio E. Grossmann: “An outer-approximation algorithm for a class of mixed-integer nonlinear programs”, *Math. Program.*, Vol. 36(3), pp. 307–339, 1986.

URL <http://dx.doi.org/10.1007/BF02592064>

This presentation presents scaled quadratic cuts based on scaling second-order Taylor expansion terms for decomposition methods, Outer Approximation (OA) and Partial Surrogate Cuts (PSC) for convex Mixed Integer Nonlinear Programming (MINLP). The scaled quadratic cut is proven to be a stricter and tighter underestimation for the convex nonlinear functions than the classical supporting hyperplanes. The scaled quadratic cut can accelerate the convergence of the MINLP methods. We integrate the presented strategies of the scaled quadratic cuts, multi-generation cuts with OA and PSC, and develop six types of MINLP solution methods with scaled quadratic cuts. We also discuss the computational implementation of the Mixed Integer Quadratically Constrained Programming (MIQCP) master problem that makes use of the Quadratically Constrained Programming (QCP) solution methods. Numerical results of benchmark MINLP problems demonstrate the effectiveness of the proposed MINLP solution methods with scaled quadratic cuts. In particular, numerical experiments show that OA and PSC with scaled quadratic cuts and multigeneration cuts can solve all the tested MINLP benchmark problems, and need few iterations and CPU solution times, especially for difficult problems.

3.15 Binary Extended Formulations for Mixed-Integer Linear Programs

Oktay Gunluk (IBM TJ Watson Research Center – Yorktown Heights, US), Sanjeeb Dash (IBM TJ Watson Research Center – Yorktown Heights, US), and Robert Hildebrand

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Main reference Sanjeeb Dash, Oktay Gunluk, Robert Hildebrand: “Binary Extended Formulations of Polyhedral Mixed-integer Sets”, *R. Math. Program.*, Vol. 170(1), pp. 207–236, Springer, 2018.

URL <https://doi.org/10.1007/s10107-018-1294-0>

URL http://www.optimization-online.org/DB_HTML/2018/01/6403.html

We analyze different ways of constructing binary extended formulations of polyhedral mixed-integer sets with bounded integer variables and compare their relative strength with respect to split cuts. We show that among all binary extended formulations where each bounded integer variable is represented by a distinct collection of binary variables, what we call “unimodular” extended formulations are the strongest. We also compare the strength of some binary extended formulations from the literature. Finally, we study the behavior of branch-and-bound on such extended formulations and show that branching on the new binary variables leads to significantly smaller enumeration trees in some cases.

3.16 Disjunctive cuts and extended formulations for bilinear functions

Akshay Gupte (Clemson University, US)

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Joint work of Akshay Gupte, Thomas Kalinowski, Fabian Rigterink, Hamish Waterer

Main reference Akshay Gupte, Thomas Kalinowski, Fabian Rigterink, Hamish Waterer: “Extended formulations for convex hulls of some bilinear functions”, CoRR, Vol. abs/1702.04813, 2017.

URL <https://arxiv.org/abs/1702.04813>

We consider the problem of convexifying a bilinear function over some bounded polyhedral domain. When the incidence graph of this function is bipartite, the convex hull is known to be polyhedral. Special structure on one set of variables in the partition can be used to characterize this convex hull. If the structure is box constraints, then we note that a sequential convexification procedure converges to the convex hull. If the structure is a simplicial polytope, i.e., a polytope whose every facet is a simplex, then we use disjunctive programming to derive a small (polynomial)-sized extended formulation of the convex hull. Our second set of results is for the non-bipartite case of the incidence graph. Here, we characterize several graphs for which a small (linear) number of inequalities that are valid for the Boolean Quadric Polytope are sufficient to obtain a minimal extended formulation of the convex hull of the bilinear function. Our proof technique uses a new measure-theoretic characterization of combinatorial polytopes that we simplify from literature and establish for graphs of nonlinear functions over boxes.

3.17 Semidefinite Programming Cuts in Gravity

Hassan Hijazi (Los Alamos National Laboratory, US)

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Joint work of Ksenia Bestuzheva, Hassan Hijazi

URL <https://www.allinsights.io/gravity>

Gravity is an open source, scalable, memory efficient modeling language for solving mathematical models in Optimization and Machine Learning. It exploits structure to reduce function evaluation time including Jacobian and Hessian computation. Gravity is implemented in c++ with a flexible interface allowing the user to specify the numerical accuracy of variables and parameters. It is also designed to handle iterative model solving, convexity detection, distributed algorithms, and constraint generation approaches. When compared to state-of-the-art modeling languages such as Jump, Gravity is 5 times faster in terms of function evaluation and up to 60 times more memory efficient. It also dominates commercial languages such as Ampl on structured models including quadratically-constrained and polynomial programs. In this talk, we will give a brief overview of the language and present preliminary results on generating linear cuts that capture the strength of semidefinite programming relaxations and their implementation in Gravity.

3.18 Stronger polyhedral relaxations for polynomial optimization problems

Aida Khajavirad (Carnegie Mellon University – Pittsburgh, US) and Alberto Del Pia (University of Wisconsin – Madison, US)

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We consider the Multilinear set defined by a collection of multilinear terms over the unit hypercube. Such sets appear in factorable reformulations of many types of mixed-integer nonlinear programs including polynomial optimization problems. Utilizing an equivalent hypergraph representation for the Multilinear set, we derive various types of facet defining inequalities for its polyhedral convex hull and present a number of tightness results based on the acyclicity degree of the underlying hypergraph. Finally, we discuss the complexity of corresponding separation problems.

3.19 Mixed-Integer Nonlinear Programming Applications: Pyomo Tools for Tailored Strategies

Carl Damon Laird (Sandia National Labs – Albuquerque, US)

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There are a number of applications in safety and critical infrastructure protection that are best represented as mixed-integer nonlinear programming problems (MINLP), having nonlinear models of the key physics and discrete decisions. These applications push the limits of general off-the-shelf solvers due to large size induced by network structure or discretization due to uncertainty or time. In this presentation, I will discuss two MINLP applications (gas detector placement in chemical process facilities and global solution of ACOFP problems) and our multi-tree solution strategies based on problem tailored relaxations and progressive refinement. We are working on a toolset within Pyomo to provide support for rapid development of these tailored solution strategies and testing of new relaxations and cuts.

3.20 Global solutions of MIQCPs

Amélie Lambert (CNAM – Paris, FR)

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We present an algorithm for solving MIQCPs. For this, we develop a B&B based on a quadratic convex relaxation of the initial problem. This relaxation is built from the solution of a semidefinite programming relaxation and captures its strength. Computational experiences show that our general method is competitive with standard solvers, on many instances. This is a dummy text.

3.21 Virtuous smoothing and more virtuous smoothing

Jon Lee (University of Michigan – Ann Arbor, US), Daphne Skipper, and Luze Xu

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Joint work of Luze Xu, Daphne Skipper, Jon Lee

I am going to talk about how to smooth a univariate increasing concave function that is nice except at 0, where the derivative maybe be intolerably large (or infinite, which is definitely computationally intolerable). The killer application is power functions $f(w) := w^p$, with $0 < p < 1$, on $[0, \infty]$; some advocate these types of functions for inducing sparsity. In the context of MINLP (where we care about being nice to NLP solvers and in producing bounds), I will explain how to do this in a nice way, with a particular increasing concave smooth piecewise-defined function that is better than a simple shift. Our results apply under very general conditions, which I won't fully reveal in a 15 minute talk. Facility to handle our methodology was introduced in SCIP. We (Luze Xu, Daphne Skipper, J. Lee) now have a paper on arXiv (see [1]).

References

- 1 Luze Xu, Daphne Skipper, Jon Lee. More virtuous smoothing.
arXiv: <https://arxiv.org/abs/1802.09112>

3.22 Mixed-Integer Derivative-Free Optimization

Sven Leyffer (Argonne National Laboratory – Lemont, US)

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Many design and engineering applications result in optimization problems that involve so-called black-box functions as well as integer variables, resulting in mixed-integer derivative-free optimization problems (MIDFOs). MIDFOs are characterized by the fact that a single function evaluation is often computationally expensive (requiring a simulation run for example) and that derivatives of the problem functions cannot be computed or estimated efficiently. In addition, many problems involve integer variables that are non-relaxable, meaning that we cannot evaluate the problem functions at non-integer points.

We present a new method for non-relaxable MIDFO that enables us to prove global convergence under idealistic convexity assumptions. To the best of our knowledge this is the first globally convergent method for non-relaxable MIDFO apart from complete enumeration. Our method constructs hyperplanes that interpolate the objective function at previously evaluated points. We show that in certain portions of the domain, these hyperplanes are valid underestimators of the objective, resulting in a set of conditional cuts. The union of these conditional cuts provide a nonconvex underestimator of the objective. We show that these nonconvex cuts can be modeled as a standard mixed-integer linear program (MILP). We provide some early numerical experience with our new method.

3.23 LP and SDP for kissing numbers

Leo Liberti (CNRS & Ecole Polytechnique – Palaiseau)

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Joint work of Jon Lee, Leo Liberti

Main reference Jon Lee, Leo Liberti: “On an SDP relaxation for kissing number”, *Optimization Letters*, pp. 1–6, Springer, 2018.

URL <https://doi.org/10.1007/s11590-018-1239-9>

Main reference Leo Liberti: “Mathematical programming bounds for kissing numbers, in Proc. of AIRO/ODS 2017, *Proceedings in Mathematics and Statistics*, Vol. 217., pp. 213–222, Springer, 2017.

URL https://doi.org/10.1007/978-3-319-67308-0_22

The “natural” MINLP formulation for the Kissing Number Problem (KNP) yields an SDP formulation for which we prove a uselessness theorem. We also look at some practical issues arising from the well known Delsarte LP bound.

3.24 External Intersection Cuts

James Luedtke (University of Wisconsin – Madison, US) and Eli Towle

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Intersection cuts are a general framework for deriving valid inequalities for nonconvex optimization problems. Specifically, given an open convex set C that does not contain any feasible solution and a basic solution that lies inside C , the intersection cut is derived by intersecting the rays of the cone K defined by the basic solution with the boundary of C , and using these points to define the separating hyperplane. Intersection cuts can be derived from both feasible and infeasible bases of a polyhedral relaxation of the problem. We investigate a new approach for deriving cuts from infeasible bases for which the basic solution does not lie in the set C (i.e., external points). Surprisingly, we find that the intersection cut framework can be used to derive valid disjunctions from such solutions, which can in turn be used to derive valid inequalities via Balas’ disjunctive cut framework. We present examples that illustrate when this framework can identify cuts that are not implied by standard intersection cuts.

3.25 Automatic reformulations of convex MINLPs in Minotaur

Ashutosh Mahajan (Indian Institute of Technology – Mumbai, IN)

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Joint work of Ashutosh Mahajan, Sharma, Meenarli

We consider two structures that may be exploited for solving convex MINLPs faster: separability in the nonlinear functions and perspective reformulations. We have implemented algorithms to identify these structures and reformulate the convex relaxation automatically. We will describe these methods and show how they were implemented in the Minotaur framework. Our experiments show that automatic reformulation can significantly reduce the solution time for benchmark instances when these structures are detected.

3.26 Optimising with Gradient-Boosted Trees and Risk Control

Miten Mistry (Imperial College London, GB), Dimitrios Letsios, Gerhard Krennrich, Ruth Misener (Imperial College London, GB), and Robert M. Lee

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Decision trees usefully represent the sparse, high dimensional and noisy nature of chemical data from experiments. Having learned a function from this data, we may want to thereafter optimise the function, e.g. for picking the best catalyst for a chemical process. This work studies a mixed-integer nonlinear optimisation problem involving:

- gradient boosted trees modelling catalyst behaviour
- penalty functions mitigating risk
- penalties enforcing chemical composition constraints.

We develop several heuristic methods to find feasible solutions, and an exact, branch and bound algorithm that leverages structural properties of the gradient boost trees and penalty functions. We computationally test our methods on an industrial instance from BASF.

3.27 Using 2D Projections for Separation and Propagation of Bilinear Terms

Benjamin Müller (Konrad-Zuse-Zentrum – Berlin, DE), Ambros M. Gleixner (Konrad-Zuse-Zentrum – Berlin, DE), and Felipe Serrano (Konrad-Zuse-Zentrum – Berlin, DE)

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One of the most fundamental ingredients in mixed-integer nonlinear programming solvers is the well-known McCormick relaxation for a bilinear product of two variables x and y over a box-constrained domain. The starting point of this talk is the fact that these may be far from tight if the feasible region and its convexification projected in the x - y -space is a strict subset of the box. We develop an algorithm that solves a sequence of linear programs in order to compute globally valid inequalities on x and y in a similar fashion as optimization-based bound tightening. These valid inequalities allow us to exploit polyhedral results from the literature in order to tighten the classical McCormick relaxation. As a consequence we obtain a convexification procedure that can exploit objective cutoff information during branch-and-bound. We use the MINLP solver SCIP to analyze the impact of the tighter relaxations on instances of the MINLPLib2.

3.28 CIA Decomposition

Sebastian Sager (Universität Magdeburg, DE)

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Solving mixed-integer nonlinear programs (MINLPs) is hard in theory and practice. Decomposing the nonlinear and the integer part seems promising from a computational point of view. In general, however, no bounds on the objective value gap can be guaranteed and

iterative procedures with potentially many subproblems are necessary. The situation is different for mixed-integer optimal control problems with binary choices that switch over time and space. Here, a priori bounds were derived for a decomposition into one continuous nonlinear control problem and one mixed-integer linear program, the combinatorial integral approximation (CIA) problem.

We generalize and extend the decomposition idea. The extension is also transferable in a straightforward way to recently suggested variants for certain partial differential equations, for algebraic equations, for additional combinatorial constraints, and for discrete time problems.

All algorithms and subproblems were implemented in AMPL for proof of concept. Numerical results show the improvement compared to standard CIA decomposition with respect to objective function value and compared to the general purpose MINLP solver Bonmin with respect to runtime.

3.29 ALAMO: Machine learning from data and first principles

Nikolaos V. Sahinidis (Carnegie Mellon University – Pittsburgh, US)

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Joint work of Alison Cozad, David Miller, Zachary Wilson

Main reference Zachary T. Wilson, Nikolaos V. Sahinidis: “The ALAMO approach to machine learning”, Computers & Chemical Engineering, Vol. 106, pp. 785–795, 2017.

URL <http://dx.doi.org/10.1016/j.compchemeng.2017.02.010>

We have developed the ALAMO methodology with the aim of producing a tool capable of using data to learn algebraic models that are accurate and as simple as possible. ALAMO relies on integer nonlinear optimization, derivative-free optimization, and global optimization to build and optimize models. We present the methodology behind ALAMO and comparisons with a variety of learning techniques, including the lasso.

3.30 Separating over the convex hull of MINL constraints

Felipe Serrano (Konrad-Zuse-Zentrum – Berlin, DE)

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Techniques for computing facets of arbitrary mixed-integer sets have had many applications. We apply the methodology to optimize over the relaxation obtained by intersecting the convex hull of every 1-row MINL relaxations of an MINLP.

3.31 Product convexification: A new relaxation framework for nonconvex programs

Mohit Tawarmalani (Purdue University – West Lafayette, US)

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Joint work of Mohit Tawarmalani, Taotao He

We develop a new relaxation that exploits function structure while convexifying a product of n functions. The function structure is encapsulated using at most d over and underestimators. We convexify the function product in the space of estimators. The separation procedure generates facet-defining inequalities in time polynomial in d for a fixed n . If the functions are non-negative, the concave envelope can be separated in $O(nd \log(d))$. Then, we extend our construction to infinite families of under and overestimators. Our relaxation procedure can be interpreted as a two-step procedure where we first express the product as a telescoping sum and in the second step apply a simple relaxation strategy. This interpretation admits various generalizations that yield various valid inequalities for nonconvex programs. We conclude by discussing techniques to generate the over and underestimators and various ways in which the proposed techniques improve and/or generalize current relaxation schemes for factorable programs.

3.32 Mixed-integer convex representability

Juan Pablo Vielma (MIT – Cambridge, US)

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Joint work of Miles Lubin, Ilias Zadik, Juan Pablo Vielma

Main reference Miles Lubin, Ilias Zadik, Juan Pablo Vielma: “Mixed-Integer Convex Representability”, in Proc. of the Integer Programming and Combinatorial Optimization – 19th Int’l Conference, IPCO 2017, Waterloo, ON, Canada, June 26-28, 2017, Proceedings, Lecture Notes in Computer Science, Vol. 10328, pp. 392–404, Springer, 2017.

URL http://dx.doi.org/10.1007/978-3-319-59250-3_32

Main reference Miles Lubin, Ilias Zadik, Juan Pablo Vielma: “Regularity in mixed-integer convex representability”, CoRR, Vol. abs/1706.05135, 2017.

URL <https://arxiv.org/abs/1706.05135>

We consider the question of which nonconvex sets can be represented exactly as the feasible sets of mixed-integer convex optimization problems (MICP). We first show a complete characterization for the case when the number of possible integer assignments is finite. We then further study the characterization for the more general case of unbounded integer variables and introduce a simple necessary condition for representability. This condition can be used to show that the set of prime numbers is not MICP representable, even though it can be represented using polynomial equations and integrality constraints. While the result for the prime numbers suggests certain regularity of MICP representable sets, we show that even for subsets of the natural numbers, MICP representable sets can be significantly more irregular than rational mixed integer linear programming representable sets. Inspired by these irregular MICP representable sets we introduce a notion of rational MICP representability and show how this notion imposes regularity to MICP representable subsets of the natural numbers, for compact convex sets and the graphs and epigraphs of certain functions. Finally, we study other notions of regularity associated to infinite unions of convex sets with the same volume. This is joint work with Miles Lubin and Ilias Zadik.

3.33 Experimentation with MINLP solver software

Stefan Vigerske (GAMS Software GmbH, DE) and Ambros M. Gleixner (Konrad-Zuse-Zentrum – Berlin, DE)

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We briefly mention some issues that frequently come up when benchmarking software that solves MINLPs. In particular, we discuss different interpretations of primal feasibility, dependence of performance on the choice of the optimality tolerance, and difficulty in defining the optimal value of a problem. By applying permutations to the order of variables and constraints, we exploit the extend of performance variability, including its dependence on the choice of optimality tolerance and whether the primal-dual integral is less prone to variability than solving time.

3.34 Integer Optimal Solutions are Sparse

Robert Weismantel (ETH Zürich, CH)

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Joint work of Iskander Aliev, Jesus De Loera, Fritz Eisenbrand, Timm Oertel, Robert Weismantel

Given a system of m equations in n variables subject to nonnegativity, how sparse is an optimal integer solution? We prove that an optimal integer solution is independent on n and in the order of $m \log(ma)$ where a is the largest absolute value of an entry of the constraint matrix. This bound is asymptotically optimal.

3.35 Combining ADAL with Factorizing the Dual to Solve SDP

Angelika Wiegele (Alpen-Adria-Universität Klagenfurt, AT)

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Joint work of Marianna De Santis, Franz Rendl, Angelika Wiegele

Main reference Marianna De Santis, Franz Rendl, Angelika Wiegele: “Using a Factored Dual in Augmented Lagrangian Methods for Semidefinite Programming”, CoRR, Vol. abs/1710.04869, 2017.

URL <https://arxiv.org/abs/1710.04869>

Using semidefinite programming has become a promising method for solving or approximating various combinatorial optimization problems. However, solving semidefinite programs is challenging due to either the large size of the matrices involved or a huge number of constraints. The most prominent methods, interior point methods, run out of memory for many practical applications.

Other algorithms for solving semidefinite problems are based on augmented Lagrangian methods using various ways of dealing with the semidefiniteness constraint. We developed such an augmented Lagrangian algorithm where we replace the semidefiniteness constraint of the dual problem by a factorization $Z = VV^t$. Using this factorization, we end up with an unconstrained (non-convex) problem in V . We then perform updates of this matrix V towards the optimal solution of Z following an alternating direction method or in the fashion of the boundary point method. We will present results for computing the theta number of a graph and computing bounds on the quadratic linear ordering problem.

3.36 Mixed-integer conic optimization and MOSEK

Sven Wiese (MOSEK ApS – Copenhagen, DK)

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Recently Lubin et al. showed that all convex instances of the nonlinear mixed-integer benchmark library MINLPLIB2 can be reformulated as conic optimization problems using 5 different cone types. These are the linear, the quadratic, the semidefinite, the exponential and the power cones. The former three cones belong to the class of symmetric cones, whereas the latter two are non-symmetric.

We call modeling with affine expressions and the five previously mentioned cone types extremely disciplined modeling. Based on Lubin et al., and on the experience at MOSEK, we claim that almost all practical convex optimization problems can be expressed using extremely disciplined modeling, making it a quite general framework. Now it is much easier to build optimization algorithms and software for extremely disciplined optimization models rather than for general (less structured) convex problems due to the limited and explicit structure. This fact is exploited in the software package MOSEK that we will discuss.

MOSEK has for many years been able to solve conic optimization problems over the symmetric cones, but in the upcoming version 9 MOSEK can also handle the two non-symmetric cones i.e. the exponential and the power cones. In this presentation we will discuss the continuous and mixed-integer conic optimizer in MOSEK. In addition, computational results, that illustrate the performance of MOSEK on problems including non-symmetric cones, are presented.

4 Working groups

4.1 Applications in Energy

The working group on applications in the energy sector, led by Alexander Martin and Frauke Liers from the University of Erlangen-Nuremberg, addressed both structural topics at the interface between engineering and optimization as well as algorithmic bottlenecks. It was agreed that mixed-integer nonlinear programming is a key paradigm for modeling and solving engineering applications both in the energy sector and beyond. However, structurally, it became clear that the engineering community puts a stronger focus on the modeling aspect, while the applied mathematics community rather values algorithmic research, a divide that is also reflected in the publication system. Algorithmically, the participants identified that the mathematical MINLP community potentially overemphasizes research on proving optimality. However, success of MINLP in engineering applications rather requires near-optimal answers quickly and robustly. The participants formulated the recommendation to adapt solver benchmarks to these needs in order to set the right incentives for solver development according to requirements in practice.

4.2 Sound experimentation with MINLP software

This working group channeled discussions on several questions that lie at the core of the seminar. Two technical presentations on Monday prepared the session thematically and summarized central questions of solver benchmarking to the entire seminar. Stefan Vigerske

from GAMS Software presented results from a series of experiments to compare how different solvers react to various experimental parameters including tolerances for feasibility and representations of models. Timo Berthold from the solver FICO Xpress highlighted particular difficulties regarding numerical stability. During the session these observations were analyzed in more detail. The participation of core developers from the MIP and MINLP solvers ANTIGONE, BARON, Couenne, Gurobi, Minotaur, SCIP and FICO Xpress resulted in a discussion on a technical level that is generally difficult to reach in a broader audience.

The main conclusions of the session were:

- the need to incorporate experimentation on permuted models as has become standard in the MIP community;
- the need to develop more informative solver output beyond optimal solutions (including sensitivity information);
- the potential usefulness of a MINLP analogue to the „MIP kappa“ measure for an a posteriori evaluation of numerical safety;
- the affirmation that conducting fair benchmarks between different solvers remains inherently difficult and users of solver software should not rely on simplistic comparisons.

Since our working group, Timo Berthold and the FICO Xpress team are already working to move the solver software discussions into practice (see [1]).

References

- 1 <https://community.fico.com/community/articles/blog/2018/05/01/numerical-challenge-accepted>

4.3 Connections between MINLP and Machine Learning

The machine learning working group was organized and led by Andrea Lodi. Dr. Lodi started the session with a presentation on the two views of machine learning and optimization/mixed integer nonlinear programming.

- *What can MINLP do for machine learning?* One great example is improved algorithm performance on classification problems where the loss function is not convex.
- *What can machine learning do for MINLP?* He described one interesting example where classical ML techniques were used to dynamically tune parameters for the commercial MINLP software CPLEX. The discussion led to other areas where ML could be used to help MINLP algorithm performance, for example in variable branching.

Matteo Fischetti then described an interesting application of mixed integer linear programming to machine learning. It is a simple but interesting observation that for a very common type of neural net activation function – the so-called ReLU – the mapping from input to output performed by a (deep) neural network can be modeled as the solution of a mixed integer program. Given a fixed network topology and weights, this gives the opportunity of optimizing over inputs to find, for example, an input to the network that is “close” to other inputs of a given class, but for which the output of the network classifies it differently. This “adversarial” approach to machine learning is important for creating robust training sets. There followed discussion on other classes of problems where MINLP could be used in ML. First, MINLP is unlikely to be the appropriate tool for one of the most important and canonical optimization problems in ML – the training of neural networks. Second, a lot of interest was generated around finding other places where one could make use of the equivalence of MIP and the neural network encoding.

To finish the working group, Dr. Oktay Gunluk from IBM described an application in symbolic regression. The algebraic operations in a grammar of valid mathematical expressions can be modeled using integer variables, so the problem of finding the optimal mathematical form of a model that best matches data, the so-called symbolic regression problem – can be modeled as a MINLP. This is an extremely interesting and challenging class of problems. To date, the MINLP technology can solve only small-sized problems.

5 Open problems

During the *Open Problem Solving Session*, we identified several areas where more research is required. We are currently working on a more extensive document to be published in the mathematical optimization community. This paper will give complete background for these questions and invite further comments from the community.

5.1 Mathematical Foundations

- *Column generation* - If we have many columns but a convex objective function, is there a notion of column generation?
- *Second-Order Cone Representation* - When is the convex hull of a semi-algebraic set second-order cone representable? Alternatively, what is the minimum number of extra variables needed for second-order cone representability?

5.2 Computing Implications

Here we focussed on the need to make MINLP solvers (and the relevant sub solvers) more reliable, by discussing:

- improving semidefinite optimization solvers, nonlinear optimization solvers working with perspective functions, and nonlinear optimization solvers in general;
- borrowing an assortment of tools from other communities, e.g. high performance computing, multiscale and multigrid methods, and logic-based methods;
- extended formulations of mathematical optimization problems and why these are so difficult to solve.

5.3 Engineering Applications

The applications where we see significant growth potential are machine learning, optimal power flow, and the pooling problem. We discussed the current barriers to being able to solve large-scale instantiations of these problems with MINLP.

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