GOR

Gesellschaft für Operations Research e.V.

Am Steinknapp 14 b, 44795 Bochum, Tel.: 0234 / 46 22 46, Fax: 0234 / 46 22 45

79th Meeting of the GOR Working Group

Practice of the Mathematical Optimization

Global Optimization

18–19 October, 2007
Physikzentrum, Bad Honnef, Germany
(www.pbh.de)

Organisation

Josef Kallrath & Alexander Lavrov
GOR AG „Praxis der mathematischen Optimierung“

Global Optimization

Global optimization techniques find their wide application in solving non-convex NLP- or MINLP-Problems. They deliver the upper and the lower bounds and allow a proof of the global optimality with any desired accuracy. In the petroleum industry, for instance, global optimization methods are known to be used for solving planning and scheduling problems containing pooling subproblems. With the help of these methods, it is possible to find all the zero points of a nonlinear equation system, which is done, for example, while determining all the stationary states of chemical reactors.

A number of commercial software packages for solving non-convex NLP- or MINLP problems have become available, which signals an ever growing usage of these techniques.

In15 talks, each of appr. 30-45 minutes, experts from practice, research institutions or software companies will present selected problem statements and the corresponding solutions.

Particular attention will be paid to contributions from practitioners who solve real industrial problems in their fields with the help of global optimization.

Confirmations for their talks have been obtained from the following speakers:

Dr. Adil Bagirov (University of Ballarat, Ballarat, Victoria, Australia)
Dr. Michael Bussieck (GAMS GmbH, Cologne, Germany)
Prof. Dr. Tibor Csendes (University of Szeged, Szeged, Hungary)
Prof. Dr. Jürgen Garloff (University of Applied Sciences, Konstanz, Germany)
Prof. Dr. Kenneth Holmström (Mälardalen University, Västeras, Sweden)
Prof. Dr. Rainer Horst (Emeritus, University of Trier, Trier, Germany)
Dipl.-Ing. Marc Jüdes (Institute of Energy Engineering, TU Berlin, Berlin, Germany)
Prof. Dr. Josef Kallrath (GOR AG Practice of Mathematical Optimization, Weisenheim am Berg, Germany)
Dipl.-Ing. Alexander Meeraus (GAMS Corp., Washington D.C., USA)
Dr. habil. Ivo Nowak (Lufthansa Systems Berlin GmbH, Berlin, Germany)
Prof. Dr. Panos Pardalos (Center of Applied Optimization, University of Florida, FL, USA)
Prof. Dr. Oliver Stein (University of Karlsruhe, Karlsruhe, Germany)
Dipl.-Math. Stefan Vigerske (Humboldt-Universität Berlin, Berlin, Germany)
Prof. Dr. Tapio Westerlund (Abo Akademi University, Turku, Finland)

Among the topics covered we see:

- Aircraft/crew scheduling
- Aircraft construction
- Cutting stock optimization in the paper and steel industry
- Colour gemstone and maneuverability problems - design centering
- Data mining
- Design optimization of energy conversion equipment
- Foundations of global optimization
- Global optimization solvers in GAMS

All in all, we expect an interesting and comprehensive survey of „Global optimization“, reflecting modern requirements, possibilities, and limitations. The official program involves a visit and a guided tour through the Adenauer Haus in Rhöndorf.

The official opening is at 10:30 on 18.10.2007. The conference dinner takes place at 19:30 on the same day. The closure of the event is scheduled for 19.10.2007, at about 17:00.

Further contributions are welcome which describe techniques or problems and provide the corresponding bounds strictly in terms of deterministic global optimization. In particular, we look forward for practice-oriented application examples and case studies where nonconvex nonlinear optimization problems are solved exactly or with guaranteed bounds.

Josef Kallrath & Alexander Lavrov

GOR

Gesellschaft für Operations Research e.V.

Am Steinknapp 14 b, 44795 Bochum, Tel.: 0234 / 46 22 46, Fax: 0234 / 46 22 45

---

79. Sitzung der GOR Arbeitsgruppe

Praxis der Mathematischen Optimierung

Global Optimization

Physikzentrum, Bad Honnef, October 18 & 19, 2007

Thursday, Oct. 18 - 2007 : 10:30 – 19:00

10:30-10:45 Opening and Welcome Session (Josef Kallrath & Alexander Lavrov)

10:45-11:30 Panos Pardalos Center of Applied Optimization, University of Florida, FL, USA
Recent Advances and Trends in Deterministic Global Optimization

11:30-12:30 Reiner Horst Universität Trier, Trier, Deutschland
Duality Bounds in Global Optimization

12:30-13:30 ------------------------- Lunch Break --------------------------------

13:30-14:15 Michael Bussieck GAMS GmbH, Cologne, Deutschland,
Alexander Meeraus GAMS Corp., Washington D.C., USA
Global Optimization with GAMS

14:15-15:00 Stefan Vigerske Humboldt-Universität Berlin, Berlin, Deutschland
LaGO - Branch and Cut for Nonconvex MINLPs

15:00-15:15 Victor Gomer Physikzentrum, Bad Honnef, Germany
Information on the Conference Center

15:15-15:45 ------------------------- Coffee Break --------------------------------

16:00-17:30 ----------------- Visit & Guided Tour: Adenauer Haus ------------------------

17:45-18:30 Tibor Csendes University of Szeged, Szeged, Hungary
Global Optimization with Tolerances and its Applications

18:30-19:15 Josef Kallrath GOR AG Praxis der math. Optimierung, Weisenheim am Berg, D
Cutting Circles and Polygons from Area-Minimizing Rectangles

19:30- Conference Dinner – Buffet; get-together in the wine-cellar
Celebrating the 79th Meeting of our GOR Working Group

Friday, Oct 19 - 2007 : 09:00 – 17:00

09:00-09:45 Adil Bagirov University of Ballarat, Ballarat, Victoria, Australia
Derivative-Free Nonsmooth Optimization and Applications

09:45-10:30 Jürgen Garloff Hochschule Konstanz, Konstanz, Deutschland
Andrew P. Smith Hochschule Konstanz, Konstanz, Deutschland
Solution of Global Polynomial Optimization Problems

10:30-10:45 ------------------------- Coffee Break --------------------------------

10:45-11:30 Ivo Nowak Lufthansa Systems Berlin GmbH, Berlin
On Solving Optimization Problems in Airline Planning and Control

11:30-12:15 Marc Jüdes Institut für Energietechnik der TU Berlin, Berlin, Deutschland
Optimizing the Configuration and Parameters of Power Plants by considering Multiple Partial Loads

12:15-13:30 ------------------------- Lunch Break --------------------------------

13:30-14:15 Oliver Stein Universität Karlsruhe, Karlsruhe, Deutschland
On Gemstones and Maneuverability Problems: Applications of Modern Design Centering Techniques

14:15-15:00 Kenneth Holmstrom Malardalen University, Sweden
Global Optimization with MATLAB/TOMLAB

15:00-15:20 ------------------------- Coffee Break --------------------------------

15:20-16:05 Tapio Westerlund Abo Akademi University, Turku, Finnland
Some Transformation Techniques in Global Optimization with Applications

16:05-16:50 Panos Pardalos Center of Applied Optimization, University of Florida, FL, USA
Global Optimization and Data Mining in Biomedicine

16:50-17:00 Final Discussion – End of the Workshop

Global Optimization with GAMS

Michael R. Bussieck
GAMS Software GmbH
Eupener Str. 135-137
D-50933 Cologne, Germany
e-mail: `mbussieck@gams.com`

and

Alexander Meeraus
GAMS Development Corp.
Washington D.C., USA
e-mail: `alex@gams.com`

The aim of Global Optimization (GO) is to find the best solution of a nonlinear problem which might have several local optima. 5 years ago GAMS started an initiative to make several GO codes (BARON, LGO, and OQNLP) providing different methods for different problem classes available to a broad audience of academic, governmental, and commercial users. 5 years later and after quiet a few lessons learned, we recently started a new round in Global Optimization. We discuss modeling system requirements for interfacing GO solvers. Besides technical challenges, key to establish new solver technology is a transparent quality assurance process. In cooperation with various solver vendors, GAMS has developed many tools for solver QA and benchmarking. As the GO solvers become more integrated with GAMS, an analysis of these solvers with the QA and benchmarking tools becomes feasible. QA plays an important role for build trust for new products. In the same way reproducible example demonstrating the power of global optimization are import. Recent books of Pinter (LGO) and Sahinidis/Tawarmalani (BARON) contain a collection of GO example models. We show an exotic application of GO with-in a branch-and-cut framework for solving a particular mixed-integer linear programming problem.

Global optimization with tolerances and its applications

Tibor Csendes

University of Szeged
Institute of Informatics
Árpád tér 2, H-6720 Szeged, Hungary
e-mail: `csendes@inf.u-szeged.hu`

We report on an earlier successful application of optimization for industrial production control and design problems. One of the two leading airplane construction firms of the world studied with which angle the graphite fiber reinforced sheets of the airplane wall should be glued together in such a way that a given rigidity is achieved and the weight or the cost is minimal. The problem can be formulated as a 5-10 dimensional complicated nonlinear optimization problem with nonlinear constraints. The set of feasibility is not connected, it can e.g. contain holes. The real challenge was however that the better the usual approximate solutions were (obtained by stochastic techniques), the larger was the chance that a not absolutely precise production result in a structure that hurts some of the constraints. In this way the security risk would increase.

With several man-years of work we have developed the methodology of optimization with tolerances. With this we were able to solve real life problems within minutes on PCs of the 1990s in such a way that the precision of the production can be given by the user, together with the accepted level of suboptimality. With a proper interval B&B framework, the algorithm is capable to provide the guarantee that the result tolerance interval contains a global minimizer point. We discuss also the theoretical results on the convergence and the correctness of the algorithms. The methodology was applied to the characterization of chaotic dynamic systems and to some civil engineering design problems too.

Solution of Global Polynomial Optimization Problems

Jürgen Garloff
HTWG Konstanz
Fachbereich Informatik
Postfach 100543, 78405 Konstanz
e-mail: `garloff@htwg-konstanz.de`

Andrew P. Smith
HTWG Konstanz
Institut für Angewandte Forschung
Postfach 100543, 78405 Konstanz
e-mail: `smith@htwg-konstanz.de`

In our talk we consider the constrained global optimization problem, where the objective function and the functions describing the inequalities are all multivariate polynomials. We solve this problem by a relaxation method in a branch and bound framework. Special emphasis is laid on the construction of lower bound functions for the polynomials involved which can be used in the relaxed problem. We present constant and affine bound functions which are based on the expansion of a multivariate polynomial into Bernstein polynomials. We show that for sparse polynomials the exponential complexity of this method can be drastically reduced. We conclude with the extension to optimization problems involving smooth functions.

Radial Basis Algorithms for Expensive Derivative-Free Black-Box Mixed-Integer Constrained Global Optimization

Kenneth Holmström
Mälardalen University
Department of Mathematics and Physics
P.O. Box 883, SE-721 23 Västerås, Sweden
e-mail: `kenneth.holmstrom@mdh.se`

Response surface methods based on kriging and radial basis function (RBF) interpolation have been successfully applied to solve expensive, i.e. computationally costly, global black-box nonconvex optimization problems. We have implemented some of these methods in the solvers *rbfSolve* and *EGO* in the TOMLAB Optimization Environment (http://tomopt.com/tomlab/). The practical performance of the RBF algorithm is sensitive to the initial experimental design, and to the static choice of target values. Methods to overcome these limitations and the development of more robust algorithms are discussed. A new adaptive radial basis interpolation (ARBF) algorithm, suitable for parallel implementation, is presented, as well as extensions of the RBF and ARBF methods to handle linear, nonlinear and integer constraints. Results so far are excellent on standard test problems.

References

[1] Björkman, M. and K. Holmström: 2000, 'Global Optimization of Costly Nonconvex Functions Using Radial Basis Functions'. *Optimization and Engineering* **1**(4), 373–397.

[2] Gutmann, H.-M.: 2001a, 'A radial basis function method for global optimization'. *Journal of Global Optimization* **19**, 201–227.

[3] Holmström, K. and M. M. Edvall: January 2004, 'CHAPTER 19: THE TOMLAB OPTIMIZATION ENVIRONMENT'. In: L. G. Josef Kallrath, BASF AB (ed.): *Modeling Languages in Mathematical Optimization.* Boston/Dordrecht/London.

[4] Holmström, K.: 2007, 'An adaptive radial basis algorithm (ARBF) for expensive black-box global optimization'. *Journal of Global Optimization.* Accepted.

[5] Holmström, K., N.-H. Quttineh, and M. M. Edvall: 2007, 'An Adaptive Radial Basis Algorithm (ARBF) for Expensive Black-Box Mixed-Integer Constrained Global Optimization'. *Optimization and Engineering.* Revised.

[6] Jones, D. R.: 2002, 'A Taxonomy of Global Optimization Methods Based on Response Surfaces'. *Journal of Global Optimization* **21**, 345–383.

[7] Regis, R. G. and C. A. Shoemaker: 2005, 'Constrained Global Optimization of Expensive Black Box Functions Using Radial Basis Functions'. *Journal of Global Optimization* **31**(1), 153–171.

Duality Bounds in Global Optimization

Reiner Horst
Universität Trier
FB IV, Mathematik
54286 Trier
e-mail: `horst@uni-trier.de`

Most of the practically successful deterministic algorithms for finding the global minimum of a multiextremal constrained nonlinear minimization problem involve Branch-and-Bound tools. For these tools, the practical success depends crucially on the quality of the lower bounds of the nonconvex terms over simple partition-sets (such as n-rectangles, n-simplices etc.). Until recently, the current opinion was that one could hardly do better than trying to construct the uniformly best convex underestimator (the so-called convex envelope). A systematic study of the use of the Lagrangian-dual, however, shows the following pleasant properties:

(i) Branch-and-Bound methods with dual bounds do always converge to a global optimum

(ii) Dual bounds are at least as good and often better than convex envelopes

(iii) For large practical problem classes the Lagrangian dual can be obtained by solving just a single linear program. Examples include packing, parametric optimization, pooling, risk management and portfolio, multicriteria optimization and others.

Struktur- und Parameteroptimierung von Kraftwerken mit mehreren Betriebspunkten
Optimizing the Structure and Continuous Parameters of Power Plants by considering Multiple Partial Loads

Marc Jüdes
Technische Universität Berlin
Institut für Energietechnik
Marchstraße 18, 10587 Berlin
e-mail: `juedes@iet.tu-berlin.de`

and

Stefan Vigerske
Humboldt-Universität zu Berlin
Institut für Mathematik
Rudower Chaussee 25, 12489 Berlin-Adlershof
e-mail: `stefan@math.hu-berlin.de`

The design optimization of complex energy conversion plants becomes more important in a liberalized energy market. Particularly when small and industrial-sized energy conversion plants (but also increasingly big power plants due to the fluctuation of the demand of electricity) have to be optimized, the consideration of the partial load performance of the power plants plays an important role. Variable operating conditions due to both changes in requested power and deteriorated components normally cause a decreased overall plant efficiency. Hence, during the design optimization of complex power plants, the partial load performance and the different partial load operation points have to be taken into account.

While the design case of a power plant defines the maximal values of mass flow rates (more precisely: the volume flow rates), temperatures and pressures, the performance of the plant changes in partial loads. The description of the plant performance at full and partial loads requires the use of nonlinear equations. The polynomials for the calculation of the thermodynamic properties such as temperatures (T), pressures (p), enthalpies (h) and entropies (s) and the equations that describe the physical principles such as Stodola's law for the description of turbine performance are examples for nonlinear equations. Also the variations of the overall heat transfer coefficients (k, heat exchangers) and the variations of the isentropic efficiencies (η_s, compressors and turbines) due to changed mass flow rates have to be considered. And finally the investment costs of the individual components have to be calculated.

In the past, different design optimization methods for complex energy conversion plants were developed and applied, e.g., exergoeconomic methods, stochastic methods (such as evolutionary algorithms) and mathematical programming approaches. Since the solution of the optimization problem is complex and time-consuming, often only a single operation point is considered during the optimization procedure of energy conversion plants. Usually the result of these optimization procedures is not a cost optimal design under a changing operating schedule. In this case even the operation in some partial load might become impossible. The few optimization methods that take the partial load behavior into account require linearized models of the problem, while binary structure variables are optimized with stochastic methods.

This article deals with the application of mathematical programming techniques and the use of a global optimizer considering the (binary) structure and the (continuous) parameter optimization of the design and operation of complex power plants with different loads. As an example, we use a simplified gas-fired cogeneration plant. The electric power output of this plant during operation ranges between 500 and 750 MW. Additional varying process steam flows can be extracted. The plant can be operated with two gas turbines and two subsequent heat recovery steam generators. Each heat recovery steam generator consists of an economizer, an evaporator and a superheater with an optional subsequent water injector to regulate the steam temperature. The heat recovery steam generators produce steam for the high pressure and the low pressure steam turbines. In addition to the design optimization (specification of binary structure variable and continuous parameters at different loads) also the maintenance strategies of existing plants have to be optimized. This plays an important role with regard to a condition-based maintenance strategy. In this example we explain the simple modifications that are necessary to apply the generated model for the optimization of maintenance decisions concerning the individual components.

The formulation of the optimization problem leads to a mixed-integer nonlinear programming (MINLP) problem which is, due to the thermodynamic and physical properties, non-convex. We used LaGO (https://projects.coin-or.org/LaGO) to solve and GAMS to formulate the problem. LaGO implements an enhanced branch and cut algorithm. Initially the algorithm approximates non-convex functions by convex underestimators. The received convex relaxation is used to generate cuts which are used for the construction and improvement of a linear relaxation. The linear relaxation provides reliable lower bounds to the global optimum and starting points for the local search for feasible solutions. A successive branching of the search space enables an improvement of the lower underestimators in the progression of the algorithm which is used for the improvement of the linear relaxation.

The objective function of the optimization task are the levelized total required revenues (TRR). The solution provided by LaGO is $TRR = 49.5$€/MWh (upper bound) while the lower bound is $TRR = 38.9$ €/MWh.

Cutting Circles and Rectangles from Area-Minimizing Rectangles

Josef Kallrath
GOR Arbeitsgruppe
Praxis der mathematischen Optimierung
Am Mahlstein 8, 67273 Weisenheim am Berg, Germany
e-mail: `josef.kallrath@web.de`

A set of circles, rectangles, and convex polygons are to be cut from rectangular design plates to be produced or from a set of stocked rectangles of known geometric dimensions. The objective is to minimize the area of the design rectangles subject to lower and upper bounds of their widths and lengths. The objects are free of any orientation restrictions.

If all nested objects fit into one design or stocked plate the problem is formulated and solved as a nonconvex nonlinear programming problem. If the number of objects cannot be cut from one plate, additional integer variables are needed to represent the allocation problem leading to a nonconvex mixed integer nonlinear optimization problem.

This is the first time that circles and arbitrary convex polygons are treated simultaneously in this context. We present exact mathematical programming solutions to both the design and allocation problem and for small number of objects to be cut we compute globally optimal solutions.

One key idea in the developed NLP and MINLP models is to use separating planes to ensure that rectangles and polygons do not overlap with each other or with one of the circles. Another important idea for considering with several resource rectangles is to develop a model formulation which connects the binary variables only to the variables representing the center of the circles or the vertices of the polytopes but not to the non-overlap or shape constraints.

We support the solution process by symmetry breaking constraints. In addition we compute lower bounds, which are constructed by a relaxed model in which each polygon is replaced by the largest circle fitting into that polygon.

We have successfully applied several solution techniques to solve this problem among them the Branch&Reduce Optimization Navigator (`BARON`) and the `LindoGlobal` solver called from `GAMS`, and a column enumeration approach with columns representing the assignments.

Good feasible solutions are computed within seconds or minutes usually during preprocessing. In most cases they turn out to be globally optimal. For up to 10 circles, we prove global optimality up to a gap of the order of 10^{-8} in short time. Cases with a modest number of objects, for instance, 6 circles and 3 rectangles, are also solved in short time to global optimality. For test instances involving non-rectangular polygons it is difficult to obtain small gaps. In such cases we are content to obtain gaps of the order of 10 percent.

Keywords: Global Optimization, mixed integer programming, cutting stock, packing, shape constraints, non-overlap constraints, design problem, assignment

On Solving Optimization Problems in Airline Planning and Control

Ivo Nowak
Lufthansa Systems Berlin GmbH
Division Airline Planning and Control
Fritschestraße 27-28, D-10585 Berlin
e-mail: `ivo.nowak@LHsystems.com`

We give an overview of the $xOPT$ optimization suite for solving crew and aircraft scheduling problems, developed at Lufthansa System Berlin. The algorithmic core of $xOPT$ is a column generation framework combined with several reduction techniques, called reduce-and-generate approach. This technique makes it possible to compute almost globally optimal solutions of huge nonlinear scheduling problems in reasonable time. We report numerical results on crew scheduling problems. Moreover, developments for crew and aircraft recovery, integrated and robust optimization are discussed. References and further information can be found at:
`http://www.lhsystems.com/topic3/topic32/r&d/index.htm`

Recent Advances and Trends in Deterministic Global Optimization

Panos M. Pardalos
Center for Applied Optimization
Industrial and Systems Engineering Department
Biomedical Engineering Department, McKnight Brain Institute
303 Weil Hall, University of Florida
PO Box 116595, Gainesville, FL 32611-6595, USA
e-mail: `pardalos@ufl.edu`
URL: `http://www.ise.ufl.edu/pardalos`

Global optimization has been expanding in all directions at an astonishing rate during the last few decades. New algorithmic and theoretical techniques have have been developed, the diffusion into other disciplines has proceeded at a rapid pace, and our knowledge of all aspects of the field has grown even more profound. At the same time one of the most striking trends in global optimization is the constantly increasing interdisciplinary nature of the field. This talk will cover the following topics: Nonconvexity and discreteness in optimization, DC (difference of convex functions) and monotonic optimization, Multiquadratic 0-1 programming and applications, Multi-variable partition approaches and Hierarchical (multi-level) optimization, Optimization with massive datasets, Supply Chain, and E-commerce.

Global Optimization and Data Mining in Biomedicine

Panos M. Pardalos
Center for Applied Optimization
Industrial and Systems Engineering Department
Biomedical Engineering Department, McKnight Brain Institute
303 Weil Hall, University of Florida
PO Box 116595, Gainesville, FL 32611-6595, USA
e-mail: `pardalos@ufl.edu`
URL: `http://www.ise.ufl.edu/pardalos`

In recent years operations research has been widely used in in many problems in biomedicine. These problems are inherently complex and very difficult to solve. In this talk we are going to focus on global optimization techniques (multi-quadratic programming) in computational neurosciences and biclustering (nonlinear fractional optimization) based data mining approaches in cancer research. In addition, several other applications will be briefly discussed.

On Gemstones and Maneuverability Problems: Applications of Modern Design Centering Techniques

Oliver Stein
Universität Karlsruhe (TH)
Fakultät für Wirtschaftswissenschaften
Schlossbezirk 13,76131 Karlsruhe
e-mail: `stein@wior.uni-karlsruhe.de`

Design centering problems deal with the inscription of a variable body into a fixed container so that, for example, the volume of the body is maximized. Applications include

- the maximal inscription of a gemstone into a rough stone to minimize the wasted material,
- the computation of lower bounds for the volume of complicated container sets by inscription of balls, like in the maneuverability problem in robotics, and
- the determination of “innermost points” of sets in order to stay away from their boundaries, like in quality control of production processes.

We present a new numerical solution method for design centering problems with irregular geometrical shapes, in particular in the absence of convexity. The focus of this method is to produce *feasible iterates*, that is, each iterate corresponds to a body which is a guaranteed subset of the container. In addition to the maximization of the body volume, here the feasibility question gives rise to a *second* optimization problem. If the latter problem is only solved to local, but not to global optimality, feasibility cannot be guaranteed. Hence, global optimization techniques have to be employed to produce feasible iterates.

To enforce feasibility, our method constructs certain convex relaxations with ideas from the alpha-BB method of global optimization. The necessary upper bounds for functions on box domains are determined using the techniques of interval arithmetic. Using standard NLP solvers for the approximating problems, at least convergence of stationary points of the approximating problems to a stationary point of the original problem can be shown, while feasibility of all iterates is warranted. Moreover, the method can be straightforwardly combined with global optimization routines for the approximating problems.

The adaptive convexification idea may not only be applied to design centering, but also to other so-called semi-infinite problems like Chebyshev approximation or robust optimization. Numerical examples illustrate the performance of the method.

LaGO - Branch and Cut for nonconvex MINLPs

Stefan Vigerske

Humboldt-Universität zu Berlin
Institut für Mathematik
stefan@math.hu-berlin.de

Mixed-Integer Nonlinear Programming (MINLP) has many applications in all areas of engineering, applied sciences, and sciences, and due to its difficulty it is a field of active research [5]. This difficulty is given by the fact that due to the presence of discrete variables and nonconvex constraints several (and often many) local minimal points of very different quality can appear, so that (stand-alone) local search methods are not applicable anymore for the localization of a global or at least "good" local optimal point. Under this aspect, algorithms for the global optimization of a nonconvex MINLP have been developed and implemented, among them the famous state-of-the-art solver BARON [10].

Common among most solvers for nonconvex MINLPs is that they require an algebraic formulation of the model that can be used to compute convex envelopes of nonconvex functions. The solver LaGO (Lagrangian Global Optimizer) [9], which we present in this talk, does not make this assumption, but can handle problems, where only methods for function evaluation and the computation of first and second order derivatives are available.

The development of LaGO has been started in the year 2000 by Ivo Nowak as a solver for mixed-integer all-quadratic problems. In a DFG project, LaGO was extended to solve nonconvex MINLPs and used to simultaneously optimize the design and operation of a complex energy conversion system [2, 3]. Since the end of 2006, LaGO is an open-source project available at COIN-OR [7]: `https://projects.coin-or.org/LaGO`.

LaGO implements an extended Branch and Cut algorithm. In the preprocessing, every function is reformulated into a block-separable form and convex envelopes are computed for each term separately. For that purpose, non-quadratic functions are first replaced by quadratic underestimators using a powerful heuristic. Quadratic functions are then replaced by convex α-underestimators as introduced by Adjiman and Floudas [1].

Finally, a linear outer approximation is constructed by linearization of the convex relaxation and generation of mixed-integer rounding cuts [8]. Thus, the generation of these two kinds of cuts allows to inherit information about both nonlinearity in the functions and integrality restrictions.

The efficiency of our method is further improved by the application of two box reduction techniques. The first is a simple constraint propagation technique based on interval arithmetic, whereas the second encloses the feasible set of the linear relaxation.

We close the talk with promising numerical results on medium size problems from the MINLPLib [4] and GlobalLib [6] including a comparision with BARON.

References

[1] Adjiman, C.S. and Floudas, C.A., “Rigorous convex underestimators for general twice-differentiable problems”, *Journal of Global Optimization*, **9**, 23–40, (1997).

[2] Ahadi-Oskui, T., “Optimierung des Entwurfs komplexer Energieumwandlungsanlagen”, *Fortschritts-Berichte VDI*, Reihe 6, Nr. **543**, (2006).

[3] Ahadi-Oskui, T., Nowak, I., Tsatsaronis, G., and Vigerske, S., “Optimizing the design of complex energy conversion systems by Branch and Cut”, *in preparation*, (2007).

[4] Bussieck, M.R., Drud, A.S., and Meeraus, A., “MINLPLib - A Collection of Test Models for Mixed-Integer Nonlinear Programming”, *INFORMS Journal on Computing*, **15(1)**, 114–119, (2003).

[5] Floudas, C.A., Akrotirianakis, I.G., Caratzoulas, C., Meyer, C.A., and Kallrath, J., “Global Optimization in the 21st Century: Advances and Challenges”, *Computers and Chemical Engineering*, **29(6)**, 1185–1202, (2005).

[6] GAMS Development Corp., “GLOBALLib”, `http://www.gamsworld.org/global/globallib.htm`.

[7] Lougee-Heimer, R., “The Common Optimization INterface for Operations Research”, *IBM Journal of Research and Development*, **47(1)**, 57–66, (2003), `http://www.coin-or.org`.

[8] Nemhauser, G.L. and Wolsey, L.A., *Integer and Combinatorial Optimization*, Wiley-Interscience New York, (1988).

[9] Nowak, I. and Vigerske, S., “LaGO - a (heuristic) branch and cut algorithm for nonconvex MINLPs”, Humboldt University Berlin, Department of Mathematics, Preprint, **06-24**, (2006), and submitted.

[10] Tawarmalani, M., and Sahinidis, N.V., “Global optimization of mixed-integer nonlinear programs: A theoretical and computational study”, *Mathematical Programming*, **99(3)**, 563–591, (2004).

Some Transformation Techniques in Global Optimization with Applications

Professor Tapio Westerlund
Abo Akademi University
Biskopsg. 8, FIN 20900 Turku, Finland
e-mail: `twesterl@abo.fi`

Bilinearities, trilinearities and more general signomial terms appear frequently in model representations for engineering optimization problems. However, even simple nonlinearities like bilinearities make a rigorous solution of such optimization problems difficult, since these nonlinearities may give rise to problems with several local optimal solutions. Generally, constraints including signomial terms may divide the feasible region into several disjoint regions, resulting in that it is very difficult to obtain optimal or even near optimal solutions with local optimization methods. Since the decisions to be taken, in many engineering optimization problems, are generally not only continuous, but also logic and discontinous, the requirements on the model representations and their solution methods are, thus, extremely high.

In this talk some transformation techniques, applicable in mixed integer global optimization, are discussed. The transformations techniques are especially useful when solving problems, including generalized signomial constraints. Such constraints can be transformed to convex form by the transformations. In addition, when the inverse transformations are approximated by piecewise linear functions, the non-convex constraints will not only be convexified but also underestimated. The latter property is especially important in global optimization, since it allows not only to convexify and to underestimate the constraints, but also to transform the non-convex problem to convex form with a feasible region overestimating the feasible region of the original one.

When the transformation techniques are applied, the original non-convex feasible region is, implicitly, divided into convex sub-regions, by this approach, and each convex sub-region is located between the breakpoints of the piecewise linear approximations of the inverse transformations.

With the given technique, a general class of non-convex MINLP (mixed integer non-linear programming) problems can be solved to global optimality. The global optimal solution of the non-convex problem is found by solving a sequence of convexified MINLP sub-problems. After each such iteration a part of the overestimated feasible region, of the original problem, is cut off, when new breakpoints are added to the piecewise linear approximations of the inverse transformations. The algorithm terminates when a solution point is sufficiently close to or within the feasible region of the original problem. The principles behind the algorithm are given and by some numerical examples it is illustrated how the global optimal solution is obtained with the approach. Finally, some examples connected to heat-exchanger network problems and trim-loss in the Finnish paper industry will be highlighted.

References

Björk K-M., Grossmann I.E. and Westerlund T. (2002). Solving Heat Exchanger Network Synthesis Problems with Non-Constant Heat Capacity Flowrates and Heat Transfer Coefficients. *AIDIC Conference Series*, **5**, 41-48, ISBN 0390-2358, Elsevier.

Harjunkoski I., Pörn R. and Westerlund T. (2001). *The Chapter:* Mixed-Integer Non-Linear Programming: The Trim-Loss Problem. In *Encyclopedia of Optimization*, C.A. Floudas and P.M. Pardalos (eds.), *Kluwer Academic Publishers*, Vol III, 379-387, ISBN 0-7923-6932-7.

Still C. and Westerlund T. (2001). *The Chapter:* Extended Cutting Plane Algorithm. In *Encyclopedia of Optimization*, C.A. Floudas and P.M. Pardalos (eds.), *Kluwer Academic Publishers*, Vol II, 53-61, ISBN 0-7923-6932-7.

Westerlund J., Hästbacka M., Kaplin J. and Westerlund T. (2007). *The Chapter :* Production and Inventory Planning for Stock Preparation in the Tissue Industry. In *Supply-Chain Optimization Volume 4: Part II*, L. Papageorgiou and M. Georgiadis (eds.), *Wiley-VCH Verlag*.

Westerlund T. (2006). *The Chapter :* Some Transformation Techniques in Global Optimization. In *Global Optimization, from Theory to Implementations*, L.Liberti and N. Maculan (eds.), *Springer*, 45-74. ISBN 0-387-28260-2.

Westerlund T. and Isaksson J. (1998). Some Efficient Formulations for the Simultaneous Solution of Trim-Loss and Scheduling Problems in the Paper-Converting Industry. *Trans.IChemE, (Part A, Chem. Eng. Res. Des.)*, **76**, 677-684.

Westerlund T. and Pörn R. (2002). Solving Pseudo-Convex Mixed Integer Optimization Problems by Cutting Plane Techniques. *Optimization and Engineering*, **3**, 253-280.