ANNUAL SEMINAR IN OPTIMIZATION AND SYSTEMS ENGINEERING 2011

The Center of Excellence in Optimization and Systems Engineering at Åbo Akademi University organizes a one-day seminar on Thursday December 8th 2011 in Auditorium Ringbom, Axelia II, Biskopsgatan 8, Åbo, Finland.

Invited speaker
Professor Ignacio Grossmann
Carnegie Mellon University, USA

Professor Ignacio Grossmann from Carnegie Mellon University is giving two invited lectures about optimization for design and operations of process systems as well as generalized disjunctive programming in the morning sessions.

Prof. Grossmann is the Rudolph R. and Florence Dean University Professor of Chemical Engineering, and former Department Head at Carnegie Mellon University. He obtained his BSc degree in Chemical Engineering at the Universidad Iberoamericana, Mexico City, in 1974, and his MSc and PhD in Chemical Engineering at Imperial College London in 1975 and 1977, respectively. After working as an R&D engineer at the Instituto Mexicano del Petróleo in 1978, he joined Carnegie Mellon in 1979. He was Director of the Synthesis Laboratory from the Engineering Design Research Center in 1988-93. He is director of the "Center for Advanced Process Decision-making" which comprises a total of 20 petroleum, chemical and engineering companies. Prof. Grossmann is a member of the National Academy of Engineering, Mexican Academy of Engineering, and associate editor of AIChE Journal and member of editorial board of Computers and Chemical Engineering, Journal of Global Optimization, Optimization and Engineering, Latin American Applied Research, and Process Systems Engineering Series. Prof. Grossmann has received a great number of awards and honors. He was named one of the "One hundred engineers of the modern era" by AIChE in 2008, and is one of the most cited authors in computer science and chemical engineering. He is doctor *honoris causa* at University of Maribor, Slovenia and Åbo Akademi University. During his career he has published in total over 350 publications and graduated over 40 PhD students.

The seminar continues in the afternoon with presentations by some of the post doc researchers and PhD students active within the Center of Excellence in OSE.

The seminar is open to anyone interested.

For registration and more information visit the OSE group's website at abo.fi/ose

OSE OPTIMIZATION AND SYSTEMS ENGINEERING

Åbo Akademi University

TIME SCHEDULE

10.00 Prof. Tapio Westerlund, chairman of the OSE group
Opening statement

10.05 Prof. Ignacio Grossmann
Discrete and continuous optimization models for the design and operation of sustainable and robust process systems

10.50 COFFEE BREAK

11.05 Prof. Ignacio Grossmann
Relaxations for convex nonlinear generalized disjunctive programs and their application to nonconvex problems

11.50 LUNCH BREAK

13.15 Andreas Lundell, PhD
A reformulation framework for global optimization

13.40 Ray Pörn, PhD
On the construction of finite Blaschke products with prescribed critical points

14.05 Henrik Nyman, PhD student
Labeled graphical models

14.25 COFFEE BREAK

14.40 Mikael Nyberg, PhD student
A novel approach to include limited equipment connectivity in state-task network models

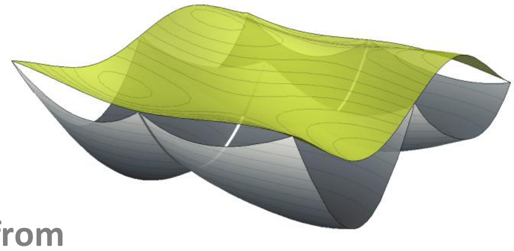
15.00 Anders Skjäl, PhD student
A generalization of classical αBB underestimation to include bilinear terms

15.20 Otto Nissfolk, PhD student
Solving rank-1 quadratic assignment problems

15.40 Axel Nyberg, PhD student
MILP formulations for the quadratic assignment problem

16.00 Amir Shirdel, PhD student
System identification by support vector regression

GLOBAL OPTIMIZATION AND ITS APPLICATIONS



At the OSE-seminar, Professor Ignacio Grossmann from Carnegie Mellon University is giving two talks connected to optimization applications in process systems engineering and generalized disjunctive programming for nonconvex optimization problems.

1. Discrete and continuous optimization models for the design and operation of sustainable and robust process systems

In this presentation we give an overview of recent applications in Process Systems Engineering of new discrete and continuous optimization techniques. We first provide a brief overview of logic-based optimization methods, emphasizing the theoretical relation of the continuous relaxations between mixed-integer programming and generalized disjunctive programming for nonconvex optimization problems. We discuss approaches for solving these problems to global optimality, with the major aim being the prediction of tight lower bounds on the global optimum. Several applications are presented to highlight the recent advances of these techniques, and their impact for improving the design and operation of sustainable and robust process systems through creative mathematical modeling. In the area of sustainable process synthesis we consider as examples the synthesis of integrated process water systems, and the energy optimization of corn-based and lignocellulosic bioethanol plants in which we also illustrate the synergy between energy and water optimization. We also consider the application of mixed-integer optimization methods in the area of process operations under uncertainty where we consider optimal design of oil and gas offshore facilities and the optimal design of reliable integrated process sites. The former problem involves uncertainties in the reservoir sizes and deliverabilities, while the latter involves uncertainties in availability of plants and equipment. Both problems have in common the goal of providing robustness to the operation of the process system.

2. Relaxations for convex nonlinear generalized disjunctive programs and their application to nonconvex problems

This presentation deals with the theory of reformulations and numerical solution of generalized disjunctive programming (GDP) problems, which are expressed in terms of Boolean and continuous variables, and involve algebraic constraints, disjunctions and propositional logic statements. We propose a framework to generate alternative MINLP formulations for convex nonlinear GDPs that lead to stronger relaxations by generalizing the seminal work by Egon Balas (1988) for linear disjunctive programs. We define for the case of convex nonlinear GDPs an operation equivalent to a basic step for linear disjunctive programs that takes a disjunctive set to another one with fewer conjuncts. We show that the strength of relaxations increases as the number of conjuncts decreases, leading to a hierarchy of relaxations. We prove that the tightest of these relaxations, allows in theory the solution of the convex GDP problem as an NLP problem. We present a guide for the generation of strong relaxations without incurring an exponential increase of the size of the reformulated MINLP. We apply the proposed theory for generating strong relaxations to a dozen convex GDPs which are solved with a NLP-based branch and bound method. Compared to the reformulation based on the hull relaxation, the computational results show that with the proposed reformulations significant improvements can be obtained in the predicted lower bounds, which in turn translates into a smaller number of nodes for the branch and bound enumeration.

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

More information about the Grossmann Research Group at Carnegie Mellon University can be found on the website ***egon.cheme.cmu.edu***

ABSTRACTS FOR THE PRESENTATIONS

Andreas Lundell, PhD

A REFORMULATION FRAMEWORK FOR GLOBAL OPTIMIZATION

In this presentation a method for solving nonconvex mixed integer nonlinear programming (MINLP) problems containing smooth functions to global optimality is presented. Instead of applying a spatial branch-and-bound strategy, reformulation techniques are utilized to obtain convex overestimations of the original nonconvex problem in an extended variable space. A sequence of these reformulated problems is then solved to obtain the global solution. For convexifying general twice-differentiable functions, an αBB-like underestimator is utilized. By introducing a convex spline underestimator instead of the original αBB underestimator it is possible to further enhance the tightness of the reformulated underestimator. The result is an easily-implementable algorithm, where no direct branching is needed, for solving a very general class of optimization problems.

Ray Pörn, PhD

ON THE CONSTRUCTION OF FINITE BLASCHKE PRODUCTS WITH PRESCRIBED CRITICAL POINTS

The problem studied in this work can be stated as: "Given *n* points in the complex open unit disk, find a finite Blaschke product of degree $n+1$ with zero derivatives at all those points". A finite Blaschke product is a rational complex-valued function, unimodular on the unit circle with all poles outside the closed unit disk and all zeros in the open disk. A Blaschke structure is a quotient of two finite Blaschke products, also unimodular on the unit circle and with at least one pole in the open disk if the quotient is not a finite Blaschke product. Our solution approach leads to a system of non-convex quadratic equations whose multiple solutions correspond to different Blaschke structures. Exactly one of the solutions corresponds to the sought finite Blaschke product.

Henrik Nyman, PhD student

LABELED GRAPHICAL MODELS

Bayesian networks and Markov networks are probably the two most commonly used graphical representations of conditional dependencies among a set of random variables. In this presentation the relatively new idea of labeled graphical models is presented. Just as the case with Markov networks, labeled graphical models use undirected graphs to convey global conditional independencies. In addition, the edges between the nodes in the graph may contain labels. These labels allow us to represent local conditional independencies or context specific independencies. This property implies that labeled graphical models can represent a larger class of multinomial distributions compared to Bayesian networks and Markov networks.

Mikael Nyberg, PhD student

A NOVEL APPROACH TO INCLUDE LIMITED EQUIPMENT CONNECTIVITY IN STN MODELS

A novel approach, called State Splitting, for including limited equipment connectivity in State-Task Network formulations is presented briefly. State Splitting, in contrast to the earlier Task-Splitting-formulation for including limited equipment connectivity, does not increase the number of binary variables and is thus computationally less demanding. Furthermore, the new approach is more flexible than its predecessor as it allows merging and splitting of batches. These facts lead to faster solution times as well as higher quality solutions. The new approach is compared to existing formulations using several test cases and solved by different MILP solvers. The computational tests indicate that State Splitting in most cases outperform the older Task Split-formulation both in regards to speed and solution quality.

Anders Skjäl, PhD student

A GENERALIZATION OF CLASSICAL αBB UNDERESTIMATION TO INCLUDE BILINEAR TERMS

The classical αBB method uses univariate quadratic perturbations, $-\alpha(x_i^U - x_i)(x_i - x_i^L)$, to convexify and underestimate smooth functions. In this presentation, it is demonstrated how the method can be generalized to include bilinear perturbation terms $\beta x_i x_j$. The new underestimator is optimally chosen from a set containing the classical underestimators as a subset. Therefore it will be at least as tight as classical αBB (the Gerschgorin variant). The new underestimator can be calculated by formulas in some common special cases. In the general case it is found by solving a linear program. Proven results describe properties of the generalized method and its relation to classical αBB.

Otto Nissfolk, PhD student

SOLVING RANK-1 QUADRATIC ASSIGNMENT PROBLEMS

Rank-1 quadratic assignment problems (QAP) are solved using mixed integer quadratic programming. The QAP is reformulated using a two-stage procedure. First, the eigenvalue decomposition is applied to rewrite the flow matrix or the distance matrix as a rank-1 matrix. Then, the quadratic convex reformulation (QCR) method is applied to convexify the quadratic terms in the objective. Using the QCR method a tight convexification and good lower bounding is achieved. Two new formulations are investigated and compared to various basic linearization techniques. Finally, results from computational experiments conducted on some special generated instances are given.

Axel Nyberg, PhD student

MILP FORMULATIONS FOR THE QUADRATIC ASSIGNMENT PROBLEM

The quadratic assignment problem (QAP) is a challenging combinatorial problem arising for example in engineering design problems such as facility layout and component placing of integrated circuits on circuit boards. The problem is NP-hard and in addition, it is considered practically intractable to solve large QAP instances to proven optimality within reasonable time limits. In this presentation a useful mixed integer nonlinear programming (MINLP) formulation of the problem as well as methods to reformulate QAPs to exact linear mixed integer programming (MIP) models are discussed. In addition, optimal results obtained with the reformulations, for some previously unsolved instances, from the quadratic assignment problem library, QAPLIB, are presented.

Amir Shirdel, PhD student

SYSTEM IDENTIFICATION BY SUPPORT VECTOR REGRESSION

Support vector regression (SVR) is a robust and powerful method for black-box system identification to determine mathematical models from measured data. An example of a challenging system identification problem to which SVR can be applied consists of the identification of switching systems with the property that their dynamical behavior may switch between a number of different modes. Identification of switching systems consists of identifying both the individual models which describe the system in the various modes, as well as the time instants when the mode changes have occurred. In this presentation support vector regression and its application to switching system identification are described, and some illustrative examples of the proposed methods are given.

The Optimization and Systems Engineering group at Åbo Akademi University is an interdisciplinary research group within the Division of Natural Sciences and Technology. Appointed a Center of Excellence within research at the university for the period 2010-2014, the group focuses on theory, methods and algorithms in systems engineering, optimization and statistics, as well as their applications in science and engineering.

For more information please contact Professor Tapio Westerlund (Process Design and Systems Engineering), Professor Göran Högnäs (Mathematics), Professor Jukka Corander (Statistics) or Professor Hannu Toivonen (Industrial Systems Engineering), or visit www.abo.fi/ose.