SEMINAR IN OPTIMIZATION AND SYSTEMS ENGINEERING

The Center of Excellence in Optimization and Systems Engineering at Åbo Akademi University organizes a one-day seminar on Wednesday November 3rd 2010 in Auditorium Salin, Axelia II, Biskopsgatan 8, Åbo, Finland.

Invited speaker
Prof. Christodoulos Floudas
Princeton University, USA

Professor Christodoulos Floudas from Princeton University is giving two invited lectures about global optimization and its applications in drug design in the morning session.

Professor Floudas is a world-renowned authority in mathematical modeling and optimization of complex systems. His research interests lie at the interface of chemical engineering, applied mathematics, and operations research. He is Professor of Chemical and Biological Engineering at Princeton University since 1994, and in 2007 he was further awarded the prestigious Stephen C. Macaleer '63 Professorship in Engineering and Applied Science at the same university. He is the author of the textbooks, Nonlinear and Mixed-Integer Optimization (Oxford University Press, 1995), and Deterministic Global Optimization (Kluwer Academic Publishers, 2000), has co-edited several monographs/books and is the chief co-editor of the Encyclopedia of Optimization (Kluwer Academic Publishers, 2001 and Springer, 2008).

The seminar continues in the afternoon with presentations, where some of the post doc researchers and PhD students present excerpts of the research currently being performed 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 **www.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

Rector Jorma Mattinen, Åbo Akademi University
Words of welcome

10.15 Prof. Christodoulos Floudas
Deterministic Global Optimization: Advances in Theory and Applications

11.15 Prof. Christodoulos Floudas
De Novo Design of Proteins and Protein-Peptide Complexes: Advances and Challenges

12.00 LUNCH BREAK

13.15 Mikael Kurula, PhD
An overview of the state/signal approach to infinite-dimensional systems theory

13.40 Ray Pörn, PhD
Three applications of semidefinite programming for 0-1 quadratic programs

14.05 Andreas Lundell, PhD
The signomial global optimization (SGO) algorithm

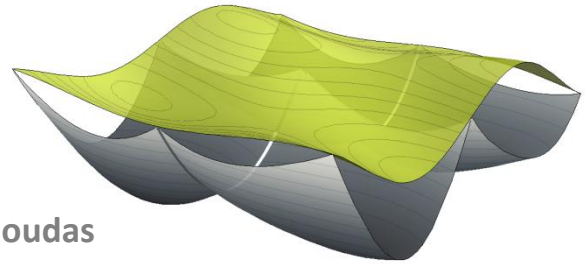
14.30 COFFEE BREAK

15.00 Anders Skjäl, PhD student
Implementation of an αBB-type underestimator in the SGO-algorithm

15.20 Henrik Nyman, PhD student
Stochastic Bayesian learning algorithm for graphical models

15.40 Mikael Nyberg, PhD student:
Modeling a complex production process using a State-Task-Network formulation

GLOBAL OPTIMIZATION AND ITS APPLICATIONS



At the OSE seminar, Professor Christodoulos Floudas from Princeton University is giving two talks about theoretical advances in and some current application areas of global optimization.

1. Deterministic Global Optimization: Advances in Theory and Applications

In this presentation, we will provide an overview of the research progress in global optimization. The focus will be on important contributions during the last five years, and will provide a perspective for future research opportunities. The overview will cover the areas of

a) twice continuously differentiable constrained nonlinear optimization, and
b) mixed-integer nonlinear optimization models.

Subsequently, we will present our recent fundamental advances in (i) convex envelope results for multi-linear functions, (ii) a piecewise quadratic convex underestimator for twice continuously differentiable functions, (iii) the generalized alpha-BB framework, (iv) our recently improved convex underestimation techniques for univariate and multivariate functions, and (v) generalized and extended pooling problems. Computational studies will illustrate the potential of these advances for important small, medium and large-scale applications.

2. De Novo Design of Proteins and Protein-Peptide Complexes: Advances and Challenges

Proteins serve as vital components in our cellular makeup and perform many biological functions that are essential for sustaining life. An important feature which determines the functionality of a protein is the form of its three-dimensional structure. Elucidated protein structures can also serve as templates for the de novo protein design which is of major importance in structure-based drug design and plays a pivotal role in the scientific challenge/roadmap: sequence to structure to function.

The primary objective in de novo protein design is to determine the amino acid sequences which are compatible with specific template backbone structures that may be rigid or flexible. It is of fundamental importance since it addresses the mapping of the space of amino acid sequences to the space of known protein folds or postulated/putative protein folds. It is also of significant practical importance since it can lead to the improved design of inhibitors, design of novel sequences with better stability, design of catalytic sites of enzymes, and drug discovery.

The first part of this presentation will provide a motivation for the de novo protein design problem with flexible backbone template structures and an overview of the advances and limitations of the existing approaches. The second part will introduce a novel two stage approach which takes into account explicitly the flexibility of the templates. The first stage addresses the in silico sequence selection problem. The second stage addresses the fold specificity by performing structure prediction calculations using atomistic level force fields and the first principles approach, Astro-Fold. The probabilities of each sequence to fold specifically to the flexible templates are calculated. The third part will introduce an approach for the prediction of approximate binding affinities in protein-peptide complexes. Prediction results for proteins and protein-peptide complexes that include variants of Compstatin, human beta defensins, C3a, inhibitors for Complement C3c, and entry inhibitors for HIV-1 will be presented.

More information about the Computer-Aided Systems Laboratory in the Department of Chemical and Biological Engineering at Princeton University can be found on the website **titan.princeton.edu.**

ABSTRACTS FOR THE PRESENTATIONS

An overview of the state/signal approach to infinite-dimensional systems theory

Mikael Kurula, PhD

I briefly present the basic concepts of the recent theory of state/signal systems in both continuous and discrete time. The talk includes an overview of the theory developed to date as well as some connections to closely related research fields. Finally, some interesting directions for future research are pointed out. We will look at a few examples if time permits.

Three applications of semidefinite programming for 0-1 quadratic programs

Ray Pörn, PhD

It is known that semidefinite programming (SDP) can be used to derive tight relaxations for a variety of hard optimization problems. In the particular case of 0-1 quadratic programs, SDP has recently been used as a reformulation tool. We also discuss how SDP can be used as a pre-processing step to obtain a reduction of the combinatorial space. The Coulomb glass is a combinatorial optimization problem that origins from physics, and appears for example in the study of semiconductors at low temperature. We formulate the Coulomb glass as a linearly constrained 0-1 quadratic program and use SDP to (i) construct tractable relaxations, (ii) create tight reformulations and (iii) obtain combinatorial reduction of the space.

The signomial global optimization (SGO) algorithm

Andreas Lundell, PhD

Global optimization of mixed integer nonlinear programming (MINLP) problems containing signomial function is often a difficult task, since signomials are often highly nonlinear and nonconvex. The signomial global optimization (SGO) algorithm can be used to solve this type of MINLP problems to global optimality as a sequence of overestimated and convexified subproblems. In the algorithm, convex underestimators for the nonconvex signomial terms are obtained using single-variable power and exponential transformations approximated with piecewise linear functions. In the presentation, in addition to a brief introduction to the SGO algorithm, some simple illustrative examples are given.

Implementation of an αBB-type underestimator in the SGO-algorithm

Anders Skjäl, PhD student

One of the few known global approaches to optimization with general twice differentiable constraints is the αBB method. The principle of the method is to convexify functions by adding parabolas in some or all of the variables. This is used in a branch and bound framework by dividing the domain in smaller hyperrectangles. An interesting question is if it is possible to use the same convexifications without branching. We have found a convex formulation where each new breakpoint is handled by one binary and one continuous variable and some adjustments in the constraints.

Stochastic Bayesian learning algorithm for graphical models

Henrik Nyman, PhD student

Automated statistical learning of graphical models from data has attained a considerable degree of interest in the machine learning and related literature. It is of great interest to develop stochastic search methods that are not prone to give local optimal models as results. For instance greedy methods are prone to yield locally optimal model structures. As most search algorithms are based on the standard Metropolis-Hastings theory, the proposal mechanisms need to be relatively simple. If we instead use a non-reversible Markov chain it is possible to utilize more intelligent proposal mechanisms, which results in methods that are less prone to get stuck in a local optimum.

Modeling a complex production process using a State-Task-Network formulation

Mikael Nyberg, PhD student

Using general modeling frameworks when formulating mathematical optimization models has many benefits. Foremost, it reduces the workload of modeling as key constraints are given by the framework. Furthermore, a general formulation such as the State-Task-Network (STN), is highly adaptable making it easier to modify the mathematical model if the system under investigation changes. On the downside a general framework can create unnecessarily large models for complex systems. In this presentation a complex production process is modeled using a STN formulation. The performance of the STN-model will then be compared to a previously developed tailor made model of the same system. The strengths and drawbacks of using general modeling frameworks for complex production problems will be discussed.

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, and their applications in science and engineering.

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