Workshop on Global Optimization: Methods and Applications

May 11-12, 2007
Fields Institute, Toronto

Organizers

Thomas Coleman (University of Waterloo)
Panos Pardalos (University of Florida)
Stephen Vavasis (University of Waterloo)

Overview

This workshop will explore recent practical progress made in the area of global optimization, especially in reference to industry applications. The program is divided into four theme areas: methodologies; algorithms and software; combinatorial and geometric applications; scientific and engineering applications. Our goal is to develop connections amongst researchers and applications workers in this area and raise awareness of current methodologies and approaches amongst practitioners.

Intended participants

The workshop is targeted to “methods” researchers in global optimization, applications researchers who use global optimization in their work, and prospective application users of global optimization. Academics will come from various disciplines: mathematics and computer science, engineering, science, and economics/finance. Industry participants can represent very diverse areas: energy-related industries, drug design and pharmaceuticals, finance and fund management, engineering design, environment resource planning…

PROGRAM

Friday, May 11, 2007

9:00 Opening remarks - Thomas F. Coleman, University of Waterloo

Methodologies

9:15 Trust-Tech Paradigm for Computing High-quality Optimal Solutions: Method and Theory - *Hsiao-Dong Chiang, Cornell University*

I will present a Trust-Tech paradigm for systematically computing multiple high-quality local optimal solutions of general nonlinear programming problems with disconnected feasible regions in a deterministic manner. Trust-Tech paradigm is composed of two distinct main phases. In Phase I, it systematically locates each feasible component of the constrained nonlinear optimization problem by exploiting trajectories of a quotient gradient dynamical system. In Phase

II, it systematically finds all the local optimal solutions located in a feasible component method by exploiting trajectories of a projected gradient dynamical system to. Specifically, starting from a feasible vector generated at Phase I, the key function of Phase II of the Trust-Tech method finds a set of surrounding local optimal solutions located in the feasible component in a tier-by-tier manner. By alternating between Phase I and Phase II of the Trust-Tech method, a set of high-quality local optimal solutions are located in a deterministic manner. A theoretical basis of the Trust-Tech method will be presented. Trust-Tech methodology has been applied to numerical large examples arising from several disciplines with very promising results.

10:00 Deterministic Global Optimization: Advances in Convex Underestimation Methods and Applications – *Christodoulos A. Floudas, Princeton University*

It is now established that Global Optimization has ubiquitous applications not only in Chemical Engineering but also across all branches of engineering, applied sciences, and sciences (e.g., see the textbook by Floudas 2000). As a result, we have experienced significant interest in new theoretical advances, algorithmic and implementation related investigations, and their application to important scientific problems.

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, (b) mixed-integer nonlinear optimization, and (c) optimization with differential-algebraic 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, and (iv) our recently improved convex underestimation techniques for univariate and multivariate functions. Computational studies will illustrate the potential of these advances.

10:45 – 11:00 Break

11:00 A Lagrangean Based Branch-and-Cut Algorithm for Global Optimization of Nonconvex Mixed-Integer Nonlinear Programs with Decomposable Structures - *Ignacio E. Grossmann, Carnegie Mellon University*

In this work we present a global optimization algorithm for solving a class of large-scale nonconvex optimization models that have a decomposable structure. Such models are frequently encountered in two-stage stochastic programming problems. A generic formulation and reformulation of the decomposable models is given. We propose a specialized deterministic branch-and-cut algorithm to solve these models to global optimality, wherein bounds on the global optimum are obtained by solving convex relaxations of these models with certain cuts added to them. These cuts are based on the solutions of the sub-problems obtained by applying Lagrangean decomposition to the original nonconvex model. Two major applications are presented to illustrate the application of the proposed method. The first deals with the optimal design of integrated process water systems with uncertainty in the load and recovery of contaminant. The second deals with optimal crude scheduling for front-end refinery operations.

Algorithms and Software

11:45 Global Optimization: Software Development and Advanced Applications – *János D. Pintér, Pintér Consulting Services Inc., Halifax*

Global optimization (GO) is aimed at finding the “absolutely best” solution in nonlinear decision models that frequently may have an unknown number of local optima. Finding such solutions numerically requires non-traditional, global scope search algorithms and software.

For over two decades, we have been developing GO algorithms followed by software implementations for (C and FORTRAN) compilers, optimization modeling environments (AIMMS, Excel, GAMS, MPL), and the scientific-technical computing platforms Maple, Mathematica, and MATLAB.

In this presentation we review the key technical background, followed by software implementation examples and a glimpse at various scientific and engineering applications.

12:30 – 2:00 **Lunch** (on your own)

2:00 Global Optimization with Branch-and-Reduce - *Nick Sahinidis, University of Illinois*

We describe theoretical and algorithmic components of the branch-and-reduce approach to the global optimization of continuous, integer, and mixed-integer nonlinear programs. These include: a theory of convex extensions for the construction of closed form expressions of convex envelopes of nonlinear functions, an entirely linear-programming-based approach to global optimization, a theory of domain reduction, and proofs of finiteness for certain branching schemes. Applications from a variety of application areas will be reviewed and extensive computational results with BARON will be reported.

Scientific and Engineering Applications

2:45 Nonlinear Integer Programming Applications in Biomedicine - *Panos M. Pardalos, University of Florida*

In recent years optimization has been widely used 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 0-1 integer programming) in computational neurosciences and biclustering (nonlinear fractional 0-1 integer programming) based data mining approaches in cancer research. In addition, several other applications will be briefly discussed.

3:30 – 3:45 **Break**

3:45 Global Optimization Issues in Parametric Programming & Control – *Vivek Dua, University College London*

The last decades have seen the rapid increase in the use of optimization- based techniques for improved design, control and operation of various types of engineering systems. A prime difficulty in applying these types of techniques to real systems and processes arises from the unavoidable presence of variations in the problem parameters such as fluctuations in uncertain inputs and measurements, or variations in inherent system properties and characteristics. These variations readily translate to deviations from the prescribed optimal point, thus, either failing to exploit fully the benefits of the optimization based solution or requiring the repetitive solution of the problem for different values of the problem parameters.

Parametric programming is a technique that determines computationally inexpensively the exact mapping of the optimal solution profile in the space of the system parameters. In this way the repetition of the problem solution is avoided, while the optimal solution can readily adapt to the system variability. In our group we have been developing algorithms for multi-parametric (mixed integer) linear, quadratic, non-linear and dynamic optimization problems that are commonly encountered in (i) optimization under uncertainty, where the uncertainties are the problem parameters, (ii) multi-level and multi-objective optimization where the different levels/objectives play the role of the parameters and (iii) model-based on-line control and optimization where the process states correspond to the parameters.

In this presentation, we will first give an overview of the mathematical foundations of multi-parametric programming for different classes of mathematical models. We will then discuss global optimization issues that arise in the context of nonlinear multi-parametric programs, bi-level and multi-level programming, as well as constrained multi-stage dynamic programming problems in robust model predictive control applications.

Combinatorial and Geometric Applications

4:30 Extremal Problems for Convex Polygons - *Pierre Hansen, HEC Montreal*

Consider a convex polygon V_n with n sides, perimeter P_n, diameter D_n, area A_n, sum of distances between vertices S_n and width W_n. Minimizing or maximizing any of these quantities while fixing another defines ten pairs of extremal polygon problems (one of which usually has a trivial solution or no solution at all). We survey research on these problems, which uses geometrical reasoning increasingly complemented by global optimization methods. Numerous open problems are mentioned, as well as series of test problems for global optimization and nonlinear programming codes.

5:15 - 6:30 pm **Reception** (in the Fields Institute Foyer)

Saturday, May 12, 2007

9:00 Min-Max Optimization on the Multiple Depot Vehicle Routing Problem - *Yinyu Ye, Stanford University*

The Vehicle Routing Problem (VRP) has been one of the central topics in optimization since Dantzig proposed the problem in 1959. A simple general model of VRP can be described as follows: a fleet of service vehicles needs to visit each client at least by one of its vehicles in a geometrical region at the minimum cost. In this talk we attempt to handle very large size multi-depot VRPs (MDVRP) in a general setting. We assume all client points are uniformly distributed in a convex region; and the goal is to minimize the maximal tour length of the fleet tours. This min-max MDVRP has not been intensively studied yet, though it has wide applications. Most known heuristics are proposed to minimize the total length all fleet tours. Rather than apply traditional local search techniques, we design simple linear programming-based and equitable partition-based methods to assign every client to a vehicle, and then generate a TSP tour for each vehicle. With a load balancing adjustment, the method can quickly produce satisfactory results.

9:45 VLSI Fixed-Outcome Floorplanning Using Convex Optimization - *Anthony Vannelli, University of Guelph*

Floorplanning is a critical step in the physical design of VLSI circuits. The input to a floorplanning tool is a netlist (a hypergraph connecting modules and edges) that provides a logical description of the chip, and the output is a floorplan that provides a physical description of the chip. Floorplanning is thus a mapping between the logical description (netlist) and the physical description (floorplan). The floorplanning optimization problem can be formulated as a global optimization problem minimizing wire length, with the area of each rectangular module fixed while the module's height and width are allowed to vary subject to aspect ratio constraints. While classical floorplanning seeks to simultaneously minimize the wire length and the total area of the floorplan without being constrained by a fixed outline for the floorplan, state-of-the-art technologies such as System-On-Chip require fixed-outline floorplanning. However, fixing the outline of the floorplan significantly increases the difficulty of the problem.

We propose a two-stage convex-optimization-based methodology for fixed-outline floorplanning that can also be applied to classical floorplanning. In the first stage, the problem is relaxed to a convex optimization problem that globally minimizes an approximate measure of wire length. Using the information obtained in the first stage, the second stage uses second-order cone optimization to finalize the floorplan by sizing the modules subject to the prescribed aspect ratios, and ensuring no overlap. The connection between the two stages is made using the relative position information gathered from the Voronoi diagram of the result of the first stage. We also propose an automatic interchange-free strategy to perform local improvements to the floorplan. To the best of our knowledge, this is the first time that a complete convex-programming-based method is used for fixed-outline floorplanning. Computational results on standard benchmarks demonstrate that the model is competitive with other well-known floorplanning techniques in the literature.

10:30 - 10:45 Break

10:45 Analysis of Greedy Approximation with Nonsubmodular Potential Function
- Ding-Zhu Du, University of Texas, Dallas

There exist many greedy approximations for various combinatorial optimization problems, such as set covering, Steiner tree, subset-interconnection designs, etc. There are also many methods to analyse them in the literature. However, all of previously known methods are suitable only for those greedy approximations with submodular potential functions. In a recent work of Du, Graham, Pardalos, Wan, Wu and Zhao, a new method is introduced to analyse a large class of greedy approximations with nonsubmodular potential functions, including some long-standing heuristics for Steiner trees, connected dominating set, and power-assignment in wireless networks. In this talk, I'll introduce this work.

11:30 Closing Remarks – Panos Pardalos, University of Florida

For more information and to register
visit http://www.fields.utoronto.ca/programs/scientific/06-07/globalopt/

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