Aegean Conferences Series−Vol. 10

AEGEAN CONFERENCES

Linking the international scientific community
Bringing the humanity scholars together

4th International Conference on Frontiers in Global Optimization

June 8-12, 2003
Nomikos Center
Santorini Greece

(cover picture)

Atlas was a Titan; son of Iapetus and Clymene and the brother of Prometheus. When the Titans were defeated, Atlas was condemned to hold the sky on his shoulders for all eternity—a mythical explanation of why the sky does not fall. Hercules shouldered the burden in exchange for Atlas fetching him the apples of the Hesperides.

GENERAL INFORMATION

Accommodations
All participants will be staying in the Santorini Image Hotel (A' class), which is located in Messaria, a short distance from Fira and 3 km from the airport.

Workshop venue
The Nomikos Conference Center is located in Fira, the capital of Santorini, overlooking the Caldera and the Santorini volcano.

Oral Presentations
An LCD projector, a projector for 2x2 inches slides and an overhead projector will be available for the oral presentations. Speakers are asked to bring their slides to the slide reception desk at least 30 min. before the beginning of the session.

Welcome Reception and Banquet
Badges are required for admission.

Island Tour
Buses for the city tour will be leaving from the Nomikos Center on Tuesday, June 10 at 2:45 p.m. The accompanying persons may be picked up at the Nomikos Center or otherwise at the Santorini Image Hotel. **Badges** are required for participation.

Lunches
Lunches will be served at the indicated times to all registered participants in the Nomikos Center. ***Badges*** are required for admission.

Tour and Travel Information
A desk operated by the personnel of our official Travel Agency,
"ERA Ltd.", 8 Alexandrou Soutsou Str., Kolonaki 10671 Athens – Greece
Tel.: 30-1-363-4944, FAX: 30-1-3631690, E-Mail: info@era.gr
will be located at the Nomikos Center and Santorini Image Hotel throughout the meeting.

The organizers gratefully acknowledge the generous help provided by Dimitrios Lambris in managing the organization of this meeting, and designing and publishing this program.

AEGEAN CONFERENCES

4th International Conference on Frontiers in Global Optimization

June 8-12, 2003

The Nomikos Center

Santorini, Greece

ORGANIZING COMMITTEE

Professor C.A. Floudas
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263
Tel.: (609) 258-4595
Fax : (609) 258-0211
E-mail: floudas@titan.princeton.edu
WEB:http://titan.princeton.edu

Professor P.M. Pardalos
Department of Industrial and Systems Engineering
Center for Applied Optimization
University of Florida
Gainesville, FL 32611
Tel.: (352) 392-9011
Fax : (352) 392-3537
E-mail : pardalos@ufl.edu
WEB: http://www.ise.ufl.edu/pardalos

PROGRAM OUTLINE

Sunday, June 8		
Registration	5:00-8:00 PM	"Santorini Image Hotel"
Welcome Reception/Dinner	8:00 PM	"Santorini Image Hotel"
Monday, June 9		
Breakfast	7:0 0 AM	"Santorini Image Hotel"
The bus will depart from the "Santorini Image Hotel" at 7:45 AM		
Registration	8:00 –2:00 PM	Nomikos Center
Organizers: Welcome and Opening Remarks	8:10 AM	Nomikos Center
Session I	8:20 AM	Nomikos Center
Coffee break	11:00 AM	Nomikos Center
Session II	11:30 AM	Nomikos Center
Lunch	2:10 PM	Nomikos Center
Dinner	8:00 PM	"Pyrgos", Pyrgos
The bus will depart from the "Santorini Image Hotel" at 7:30 PM		
Tuesday, June 10		
Breakfast	7:00 AM	"Santorini Image Hotel"
The bus will depart from the "Santorini Image Hotel" at 7:45 AM		
Session III:	8:20 AM	Nomikos Center
Coffee break	11:00 AM	Nomikos Center
Session IV:	11:30AM	Nomikos Center

Lunch	2:00 PM	Nomikos Center
Island Tour	2:45 PM	

Wednesday, June 11

Breakfast	7:00 AM	"Santorini Image Hotel"

The bus will depart from the "Santorini Image Hotel" at 7:45 AM

Session V:	8:20 AM	Nomikos Center
Coffee break	11:00 AM	Nomikos Center
Session VI:	11:30 AM	Nomikos Center
Lunch	2:30 PM	Nomikos Center
Dinner	8:00 PM	"Selene, Fira"

The bus will depart from the "Santorini Image Hotel" at 7:30 PM

Thursday, Juene 12

Breakfast	7:00 AM	"Santorini Image Hotel"

The bus will depart from the "Santorini Image Hotel" at 7:45 AM

Session VII:	8:20 AM	Nomikos Center
Coffee break	11:00 AM	Nomikos Center
Session VIII:	11:30 AM	Nomikos Center
Lunch	2:30 PM	Nomikos Center
Gala Dinner	8:00 PM	Nomikos Center

The bus will depart from the "Santorini Image Hotel" at 7:30 PM

Friday, Friday 13

Breakfast	7:30 AM	"Santorini Image Hotel"

Departure

PROGRAM

4th International Conference on Frontiers in Global Optimization

June 8-12, 2003
Santorini, Greece

Sunday, June 8

5:00-8:00 PM ***Open Registration*** – "Santorini Image Hotel"
8:00 PM ***Welcome Reception –*** "Santorini Image Hotel"

Monday, June 9

7:00 AM **Breakfast**
The bus will depart from the "Santorini Image Hotel" at 7:45 AM

8:00 AM-2:00 PM ***Registration*** – Nomikos Center

8:10 AM-8:20 PM **Organizers: Welcome and Opening Remarks**

Session I

Chairs: C.A. Floudas and P.M. Pardalos

8:20 AM **1** ***Applications of Nonconvex Quadratic Programming***
C. Audet, P. Hansen, and S. Le Digabel

8:40 AM **2** ***Convex Lower Bound Functions for Polynomials and Their Use in Global Optimization***
J. Garloff, C. Jansson, and A. P. Smith

9:00 AM **3** ***Lipschitz Global Optimization and Local Information***
Y. D. Sergeyev

9:20 AM **4** ***Geometric Terrain Methodologies for Global Optimization***
A. Lucia and P. A. DiMaggio

9:40 AM **5** ***D.C. Programming and Optimal Selection of the Radial-Basis Kernel Parameter***
T. B. Trafalis and A. M. Malyscheff

10:00 AM **6** ***Calibration of the Cavariance Matrix in Finance for Stable and Robust Portfolio Selection***
V. Guigues

10.20 AM **7** ***Global Optimization in Informatics***
N. V. Sahinidis

10:40 AM **8** ***A Multi-dimensional Assignment Formulation For New Product Development Problems***
R. A. Murphey

11:00 AM **Coffee Break**

Session II

Chairs: P. Hansen and F. Zirilli

11:30 AM **9** ***A Geometric Build-Up Approach to Molecular Distance Geometry Problem***
Z. Wu

11:50 AM **10** ***Global Optimization Methods for Large Scale Molecular Optimization: from Cluster Optimization to Protein-Protein Docking***
B. Addis, M. Locatelli, and F. Schoen

12:10 PM **11** ***A New Algorithm for the Global Optimization of a Computer Aided Molecular Design Model***
E. Luke, K. Achenie, and G. M. Ostrovsky

12:30 PM **12** ***Multiobjective Optimization Considerations in Metabolic Engineering***
C.D. Maranas

12:50 PM **13** ***Reducing the Cost of Evaluation of the gradient and the Hessian of Molecular Potential Energy Fuctions***
C. Lavor, N. Maculan

1:10 PM **14** ***Global Optimization of Bioprocesses using Stochastic and Hybrid Methods***
J. R. Banga, C. G. Moles, and A. A. Alonso

1:30 PM **15** ***The Steiner Ratio and Homochirality of Biomacromolecular Structures***
R. P. Mondaini and N. V. Oliveira

1:50 PM **16** ***Global Optimization Under Nonlinear Restrictions by using Stochastic Perturbations of the Projected Gradient***
J. E. Souza de Cursi, R. Ellaia, and M. Bouhadi

2:10 PM **Lunch**

8:00 PM **Dinner** "Pyrgos", Pyrgos
The bus will depart from the "Santorini Image Hotel" at 7:30 PM

Tuesday, June 10

7:00 AM **Breakfast**

The bus will depart from the "Santorini Image Hotel" at 7:45 AM

Session III

Chairs: C. Adjiman and M. Stadtherr

8:20 AM **17** ***On Gradient Flows in Global Optimization***
H. Th. Jongen

8:40 AM **18** ***Global Optimization of Bilevel Programming Problems Via Parametric Programming***
E. N. Pistikopoulos, V. Dua, and J. H. Ryu

9:00 AM **19** ***Algorithms for Quadratic Programming withSimple Bounds***
P. L. De Angelis, P. Festa, and G. Toraldo

9:20 AM **20** ***Analysis of Non Convex Polynomial Programs by the Method of Moments***
R. J. Meziat

9:40 AM **21** ***A Global Smoothing Algorithm for Global Optimization and its Applications***
W. Murray

10:00 AM **22** ***Deterministic Global Optimization in Operations Research***
C. Y. Gau and L. Schrage

10:20 AM **23** ***Global Optimization Techniques for the Eigencomplementarity Problem***
J. Judice, I. Ribeiro, and H. Sherali

10:40 AM **24** ***The Generalized aBB Global Optimization Approach: Tight convex underestimators***
I. G. Akrotirianakis and C. A. Floudas

11:00 AM **Coffee Break**

Session IV

Chairs: A. Lucia and C. Maranas

11:30 AM **25** ***Combinatorial and Continuous Approaches to the Max-Clique Problem***
I. Bomze, M. Locatelli, and M. Pelillo

11:50 AM **26** ***Analytic Centers Cutting Plane Methods and Mixed Integer Programming, with Extensions to Semi-definite Cuts***
J. L. Goffin, S. Elhedhli, M. R. Oskoorouchi

12:10 PM **27** ***Discrete and Continuous Global Optimization in Operations Research with the Variable Neighborhood Search Metaheuristic***
N. Mladenovic

12:30 PM **28** ***Some Connections Between Discrete and Continuous Optimization Problems***
F. Tardella

12:50 PM **29** ***Optimization Problems in Massive Graphs***
P. M. Pardalos, V. Boginski, and S. Butenko

1:10 PM **30** ***Exact Parallel Algorithm for Computing Maximum Feasible Subsystems of Linear Inequalities***
V. Rosta and K. Fukuda

1:30 PM **31** ***MINLP Optimization Framework Using Simplicial Approximation***
M. Ierapetritou and V. Goyal

2:00 PM **Lunch**

2:45 PM **Island Tour**

Wednesday, June 11

7:00 AM **Breakfast**
The bus will depart from the "Santorini Image Hotel" at 7:45 AM

Session V

Chairs: M. Locatelli and J. Júdice

8:20 AM **32** ***Global Optimization for Oil Reservoir Modelling***
S. Gómez, L. Castellanos, and N. del Castillo

8:40 AM **33** ***Exact Computation of Global Minima of a Nonconvex Portfolio Optimization Problem***
J. Kallrath

9:00 AM **34** ***Global Reliability-Based Design Optimization (Theory and Application)***
G. Kharmanda, A. El -Hami and N. Olhoff

9:20 AM **35** ***Generator of Classes of Test Functions for Global Optimization Algorithms***
D. E. Kvasov M. Gaviano, D. Lera, and Y. D. Sergeyev

9:40 AM **36** ***The Hinge Fitting Problem***
M. Queiroz, C. Humes Jr., and J. Júdice

10:00 AM **37** ***A General Framework for Constructing Cooperative Global Optimization Algorithms***
X. Huang

10:20 AM **38** ***A Multi-Start Methodology for Constrained Global Optimization Using Novel Constrained Local Optimizers***
J. A. Snyman, H. P. J. Bolton and A. A. Groenwold

10:40 AM **39** ***Representation and Numerical Determination of the Global Optimizer of a Continuous Function on a Bounded Domain***
J. E. Souza de Cursi

11:00 AM **Coffee Break**

Session VI

Chairs: P. Barton and F. Schoen

11:30 AM **40** ***Advances in Interval Methods for Deterministic Global Optimization in Chemical Engineering***
M. A. Stadtherr and Y. Lin

11:50 AM **41** ***Efficient Use of Gradient Information in Multidimensional Interval Global Optimization Algorithms***
L. G. Casado, J. A. Martinez, I. Garcia, Ya. D. Sergeyev and B. Toth

12:10 PM **42** ***A New Subinterval Selection Technique in Interval Global Optimization***
T. Csendes

12:30 PM **43** ***Probabilities, Intervals, What Next? Optimization Problems Related to Extension of Extension of Intercal Computations to Situations with Partial Information about Probabilities***
V. Kreinovich

12:50 PM **44** ***Termination Criteria in the Moore-Skelboe Algorithm for Global Optimization by Interval Arithmetic***
M. H. van Emden and B. Moa

1:10 PM **45** ***Matching Stochastic Algorithm to Objective Function Landscape***
W. P. Baritompa, M. Dur, E. M. T. Hendrix, M. Locatelli, L. Noakes, W. J. Pullan, and G. R. Wood

1:30 PM **46** ***Stochastic Adaptive Search Methods Based on Hit-and-Run Sampling for Discrete and Continuous Global Optimization***
Z. B. Zabinsky and Y. Shen

1:50 PM **47** ***Optimizing the Global Random Search Methods Based on Statistical Inference about the Objective Function***
A. Zhigljavsky and A. Zilinskas

2:10 PM **48** ***A One Dimensional Global Optimization Algorithm for Observations with Noise***
A. Zilinskas and J. M. Calvin

2:30 PM **Lunch**

8:00 PM **Dinner** "Selene, Fira"
The bus will depart from the "Santorini Image Hotel" at 7:30 PM

Thursday, June 12

7:00 AM **Breakfast**
The bus will depart from the "Santorini Image Hotel" at 7:45 AM

Session VII

Chairs: N. Sahinidis and Z. Zabinsky

8:20 AM **49** ***Global Optimization of Homogeneous Forms***
L. Faybusovich

8:40 AM **50** ***An Interior Point Heuristic for the Hamiltonian Cycle Problem Via Markov Decision Processes***
V. Ejov, J. A. Filar and J. Gondzio

9:00 AM **51** ***On a Class of Quasi-Hemivariational Inequalities***
Z. Naniewicz

9:20 AM **52** ***Quasiconvexity, Fractional Programming and Extremal Traffic Congestion***
C. E. M. Pearce

9:40 AM **53** ***Global Solution of Optimization Problems with Dynamic Systems Embedded***
P. I. Barton and A B. Singer

10:00 AM **54** ***A Deterministic Global Optimization Algorithm for Problems with Nonlinear Dynamics***
C.S. Adjiman and I. Papamichail

10:20 AM **55** ***New Results in Deterministic Global Optimization for Problems with Ordinary Differential Equations***
B. Chachuat and M.A. Latifi

10:40 AM **56** ***Global Dynamic Optimization of Linear Hybrid Systems***
C. K. Lee and P. I. Barton

11:00 AM **Coffee Break**

Session VIII

Chairs: C.A. Floudas and P.M. Pardalos

11:30 AM **57** ***Routing in Optical and Circuit-Switched Networks***
A. E. Ozdaglar and D. P. Bertsekas

11:50 AM **58** ***The use of global optimization in the study of data fusion***
F. Zirilli

12:10 PM **59** ***An Efficient Algorithm for the Minkowski Addition of Convex Polytopes***
K. Fukuda

12:30 PM **60** ***Effective Local Search Algorithms for the Vehicle Routing Problem with General Time Window Constraints***
T. Ibaraki, S. Imahori1, M. Kubo, T. Masuda, T. Uno and M. Yagiura

12:50 PM **61** ***Applying Global Optimization to enhance Graph Theory: The AutoGraphiX 1 and AutoGraphiX 2 Systems***
G. Caporossi and P. Hansen

1:10 PM **62** ***Exact and Heuristic Approaches for a Cyclic Delivery Problem***
P. Festa and R. Cerulli

1:30 PM **63** ***A Reliable Computer Method for the ``Packing Circles in a Unit Square'' Problems***
M. C. Markot and T. Csendes

1:50 PM **64** ***A Decomposition-Based Algorithm to the Water Irrigation Network Design Problem***
G. M. Gonçalves and M. V. Pato

2:10 PM **65** ***A Fuzzy Partitioning Based Pre-Screening Method for Improved Search Efficiency in Global Optimization***
L. Ozdamar, M. B. Demirhan, E. Onbasioglu

2:30 PM **Lunch**

8:00 PM **Gala Dinner**
The bus will depart from the "Santorini Image Hotel" at 7:30 PM

Friday, June 13

7:30 AM **Breakfast**

Departure

ABSTRACTS

ABSTRACT #1

APPLICATIONS OF NONCONVEX QUADRATIC PROGRAMMING

C. Audet[1,2], P. Hansen[1,3] and S. Le Digabel [2]
[1]GERAD, [2]Ecole Polytechnique Montreal [3]HEC Montreal

Recent applications of the Branch and Cut algorithm for nonconvex quadratic programming with nonconvex quadratic constraints of Audet, Hansen, Jaumard and Savard (Mathematical Programming 2000) are reviewed. They cover a variety of fields including geometry (the largest small octogon), production (the pooling problem), logistics and pricing (supply chain management), finance (optimizing with sum or products or ratios) and economic planning (fractional goal programming).

CONVEX LOWER BOUND FUNCTIONS AND THEIR USE IN GLOBAL OPTIMIZATION

J. Garloff, C. Jansson°, and A. P. Smith**
**University of Applied Sciences/FH Konstanz,*
°Technical University Hamburg-Harburg, Germany

We address the construction of convex lower bound functions for multivariate polynomials. They are obtained in a natural way if we represent the given polynomial p of degree n as a linear combination of the Bernstein polynomials of degree n. The coefficients of this expansion, the so-called Bernstein coefficients, can easily be computed from the coefficients of p. A fundamental property of the Bernstein expansion is its convex hull property which states that the graph of p over a box is contained in the convex hull of the control points associated with the Bernstein coefficients. Based on this property, convex lower bound functions of increasing complexity can be constructed. In the univariate case, an affine lower bound function is obtained by the facet passing through a control point with smallest Bernstein coefficient and having a slope which is smallest in absolute value under the slopes of the facets passing through this exposed vertex.

In the multivariate case the affine lower bound function c is obtained as optimal solution of a LP. We present an upper bound for the difference $p - c$ which exhibits in the univariate case quadratic convergence w.r.t. the width of the interval. Moreover, we also give some suggestions for the way in which the calculations have to be performed so that the results are guaranteed also in the presence of rounding errors.

In the second part of our talk we apply these bound functions in a branch and bound framework for solving the constrained global optimization problem in the case where the objective function and the functions describing the constraints are all polynomials.

LIPSCHITZ GLOBAL OPTIMIZATION AND LOCAL INFORMATION

Y. D. Sergeyev
University of Calabria (Italy) and University of Nizhni Novgorod (Russia)

In this talk, the constrained Lipschitz global optimization problem is considered. It is supposed that the objective function is 'black box', non-differentiable, multiextremal, and requiring a high time to be evaluated. Constraints are given by multiextremal and non-differentiable functions that can lead to complex feasible regions consisting of disjoint non-convex sub-regions. Lipschitz constants are unknown both for the objective function and the constraints which may be also partially defined, i.e., if a constraint is not satisfied at a point, the rest of constraints and the objective function may not be defined at that point.
A new powerful tool - local tuning on the behaviour of the objective function and constraints - is used to accelerate the search. It is shown that Lipschitz methods working with global estimates of the Lipschitz constants (the same estimates are used over the whole search region for the objective function and constraints) may provide a poor information about the behavior of the objective function over every small sub-region of the search domain. It is established for different classes of global optimization problems, that local tuning accelerates the search significantly.

GEOMETRIC TERRAIN METHODOLOGIES FOR GLOBAL OPTIMIZATION

A. Lucia and P. A. DiMaggio
Department of Chemical Engineering, University of Rhode Island, Kingston, RI, USA

Global optimization remains an important area of active research. Many macroscopic and microscopic applications in science and engineering still present a formidable challenge to current global optimization techniques. In this work, a completely different, novel and general geometric framework for continuous global optimization is described. The proposed methodology is based on intelligent movement along the valleys and ridges of an appropriate objective function using downhill, local minimization calculations defined in terms of Newton-like differential equations and uphill integration of the Newton-like vector field combined with intermittent SQP corrector steps. Unique features of the proposed methodology include new rigorous mathematical definitions of valleys and ridges, the combined use of objective function and gradient surfaces to guide movement, and saddle point covering techniques to assist both exploration and termination. Collisions with boundaries of the feasible region, integral curve bifurcations, and the presence of non-differentiabilities are also discussed. A variety of examples, some animated, are used to make key concepts clear and to demonstrate the reliability, efficiency and robustness of terrain methods for global optimization.

OPTIMAL SELECTION OF THE REGRESSION KERNEL MATRIX WITH SEMIDEFINITE PROGRAMMING

T. B. Trafalis and A. M. Malyscheff
School of Industrial Engineering, University of Oklahoma, Norman, Oklahoma, USA

Support vector machines have recently attracted much attention in the machine learning and optimization communities for their remarkable generalization ability. An open problem, however, is the selection of the optimal kernel matrix for regression problems. Recently, a means to compute the optimal kernel matrix for pattern classification using semidefinite programming has been introduced. In this paper we extend these thoughts to the regression analysis scenario. Preliminary experimental results are presented for which the optimal kernel matrix for support vector machine regression is retrieved.

CALIBRATION OF THE COVARIANCE MATRIX IN FINANCE FOR STABLE AND ROBUST PORTFOLIO SELECTION

V. Guigues
LMC

In this paper, we present a method improving the stability of the solutions of Markowitz problem as well as robust counterparts of this problem. To get the stability of the portfolios, a novel calibration of the covariance matrix of the returns is proposed. This calibration can be cast as a semidefinite program. To justify this calibration, we determine 2 properties that the covariance matrix should check. First, a sensitivity analysis of Markowitz model shows us the role played by the lowest eigenvalue of this matrix. Using methods inspired from this sensitivity analysis we also provide a sensitivity analysis for a Value-at-Risk problem. Second, a stochastic analysis permits us to localize the covariance matrix and the mean return vector in bounded areas and shows us how close the composition, the return and the variance of our estimated portfolio will be from the same values computed for the true portfolio. As for the robustification of the model, it is derived from the stochastic analysis which allows us to easily implement different robust counterparts of Markowitz model. The robust counterparts are second order cone programs, solved as efficiently as the nominal problem.

1. Worst case Value-at-Risk and Robust Asset Allocation : a Semidefinite Programming Approach. L.El Ghaoui, F.Oustry, M.Oks.
2. Perturbation Analysis of Optimization Problems. Springer Series in Operations Research. J.F Bonnans, A. Shapiro.
3. Robust solutions to uncertain linear programs via Convex Programming. Operations Research Letters. A.Ben-Tal, A.Nemirovski.

GLOBAL OPTIMIZATION IN INFORMATICS

N. V. Sahinidis
University of Illinois at Urbana-Champaign

With the recent accumulation of vast amounts of chemical, biological, and clinical data, many scientific fields are becoming increasingly data-driven as opposed to model-driven. This paradigm shift has brought about many challenging computational problems. Even though these problems originate from very disparate fields, they have very similar mathematical structures. In particular, they involve the use of a merit function to evaluate alternatives from very large, combinatorial search spaces.

We address the challenging informatics problems of: (a) using group contribution data to design chemicals with desired properties, (b) using x-ray diffraction data to infer three-dimensional structures of crystals, and (c) using data from fine needle aspirates to diagnose patients for breast cancer. For each problem, we present novel mathematical programming models and algorithms for their solution.

The main conclusion of the paper is that branch-and-reduce algorithms for the global optimization of the underlying models have now reached the level of maturity required to solve realistic informatics problems.

A MULTI-DIMENSIONAL ASSIGNMENT FORMULATION FOR NEW PRODUCT DEVELOPMENT PROBLEMS

R. A. Murphey
Air Force Research Laboratory, Eglin AFB, FL USA

This paper considers the application of a global heuristic and lower bounding technique to new product development (NPD) problems. NPD procedures are increasingly being used by many high-technology firms to rapidly develop multiple new products lines using a small but flexible workforce and infrastructure. Mathematically speaking, these problems are quite difficult and may be described as the allocation of heterogeneous resources to heterogeneous but perhaps interdependent activities. Typically, each resource may distribute its capacity among many activities, each resource is capable of processing more than one type of task to varying degrees of success, and activities may be processed by more than one resource either sequentially or simultaneously. One of the most complicating characteristics of NPDs is that of precedence constraints, where sequencing, quite often in the form of simultaneity, for the beginning and ending of activities is carefully controlled while processing times and quality of services for resources are not independent. Network models for these problems are very difficult to pose since, unlike PERT, there are multiple projects, all interlinked with precedence. Consequently, a multi-dimensional assignment problem (MAP) formulation is proposed. Unfortunately, MAP data structures exhibit horrendous complexity for branch and bound and cannot be solved for problems of even fairly small size. By applying a heuristic shown to be successful for other types of multi-dimensional assignment problems good solutions may be obtained. This is confirmed by a lower bound problem, which is readily developed by exploiting a feature of the cost coefficients.

A GEOMETRIC BUILD-UP APPROACH TO MOLECULAR DISTANCE GEOMETRY PROBLEM

Z. Wu
Department of Mathematics, Iowa State University, Ames, Iowa, USA

A protein structure can be determined by solving a molecular distance geometry problem with a set of inter-atomic distances or their restraints obtained from nuclear magnetic resonance experiments or other sources. The molecular distance geometry problem is polynomial-time solvable if the exact distances are given for all pairs of atoms. However, the problem is NP-hard intractable in general if only a subset of all distances is available. A novel approach to the problem is discussed in the talk. In this approach, a build-up algorithm is used to determine the coordinates of the atoms, one at a time, with the given distances between the determined atoms and the underdetermined ones, and the determination of the coordinates of each atom requires only the solution of a small linear system of equations or convex optimization problem. The approach is applicable to different types of molecular distance geometry problems, including the problems with exact distances, sparse sets of distances, and sparse inexact distances. In the ideal case when the exact distances for all pairs of atoms are given, the coordinates of n atoms can be determined by this approach in order of n floating-point operations, while in a conventional singular value decomposition approach in order of n^2 to n^3 floating-point operations. The algorithms for each different type of problems are described. Results from using the algorithms for the determination of the structures of a set of proteins and polypeptides are presented.

GLOBAL OPTIMIZATION METHODS FOR LARGE SCALE MOLECULAR OPTIMIZATION: FROM CLUSTER OPTIMIZATION TO PROTEIN-PROTEIN DOCKING

Bernardetta Addis[1], Marco Locatelli[2], ad Fabio Schoen[1]
[1]Dip. Sistemi e Informatica - Università di Firenze, Firenze (Italy)
[2]Dip. Informatica - Università di Torino, Torino (Italy)

In this paper a framework for large scale global optimization of molecular conformation problems will be presented; we will discuss some general characteristics of these problems which can be used to guide the search towards a global optimum. The numerical results obtained by our group in confirming the putative global optima of Lennard-Jones and Morse clusters by means of unbiased stochastic optimization confirm that the inclusion of some general knowledge on the problem domain can yield dramatic improvements. We obtained the configuration of the most difficult clusters with a computational effort (number of local searches) which is one to two order of magnitude less than the best published results. These encouraging results prompted us to attempt even more challenging problems. In particular we started some experiments in protein-protein docking, i.e. the problem of determining the minimum energy coupling of two complex macromolecules which interact through Van der Waals and electrostatic forces. Our first results with the simplified model of rigid docking, (where both molecules are considered to be rigid), are extremely encouraging. Rigid docking is a low-dimensional problem, but the objective function is composed of millions of pair contributions, and not only it is computationally expensive, but also it displays an enormous number of local optima. We will present some results obtained with protein complexes obtained from the PDB databank.

A NEW ALGORITHM FOR THE GLOBAL OPTIMIZATION OF A COMPUTER AIDED MOLECULAR DESIGN MODEL

E. Luke, K. Achenie and G. M. Ostrovsky
Department of Chemical Engineering, University of Connecticut, USA

In this presentation, we consider the molecular design problem modeled as a mixed-integer nonlinear programming problem (Churi and Achenie, 1996) and the global solution of such a model. The model has a relatively large number of linear constraints and a few nonlinear/non-convex constraints. The number of binary variables, characterizing the structure of a molecule can be quite large.

For solution of the MINLP, the use of the conventional BB method that does branching with respect to all the binary variables can be computationally intensive. To address this issue, we propose the reduced dimension branch and bound (RDBB) method, which differs from the conventional BB method in the way branching is implemented and how linear under-estimators are constructed. Thus, instead of branching with respect to all the binary variables in the conventional BB method, the RDBB method does branching using *branching functions*. In the suggested approach, enforcement of the integrality of all the binary variables is carried out at each iteration.

We have developed the sweep method for constructing linear under-estimators and branching functions. The method is based on a reduction of the objective function and constraints to a special tree function (STF) form that represents a superposition of concave (convex) univariate functions connected by simple arithmetic operations namely addition, subtraction, and multiplication by a scalar. Using the STF the sweep method constructs a linear under-estimator through a multilevel procedure. It is important to note that when linear under-estimators are employed, the dimension of the lower bound problem is the same as the dimension of the original problem. In contrast, the use of separable programming technique (Pantelides, 1996) will result in a significant increase in the dimension of the lower bound problem since each product of search variables and nonlinear univariate function requires the introduction of new search variables.

References

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MULTIOBJECTIVE OPTIMIZATION CONSIDERATIONS IN METABOLIC ENGINEERING

C. D. Maranas
The Pennsylvania State University, Department of Chemical Engineering
University Park,USA

In this talk, multiobjective optimization is used to gain valuable insight into two separate challenges in metabolic engineering. First, a bilevel programming approach, termed OptKnock, is applied to identify gene knockout strategies for coupling biochemical production with biomass formation. The idea here is to prune the original network so as while it maximizes an internal cellular objective, for example biomass formation, it also indirectly maximizes the production of the desired biochemical. An elegant solution strategy founded on concepts from LP duality theory is discussed. This framework is applied to (i) 1,3-propanediol, (ii) succinate, and (iii) lactic acid production in *E. coli*. Knockout strategies coupling maximum biomass formation with biochemical yields approaching 90% of their theoretical limits are introduced. Second, a similar bilevel optimization framework, ObjFind, is applied to assess whether a hypothesized cellular objective is consistent with a set of experimentally derived metabolic fluxes. Experimental flux values obtained from an *Escherichia coli* isotopomer analysis study for aerobic and anaerobic growth conditions are used in conjunction with a stoichiometric model of *E. coli* central metabolism. Specifically, we attempt to find whether there exists a weighted sum of cellular objectives (i.e., biomass formation, ATP production, etc.) whose maximization leads to a set of fluxes that match the experimental measurements. Interestingly, for both growth scenarios, the identified coefficients are almost identical suggesting a unique metabolic driving force under both conditions with the dominant coefficient corresponding to the cellular flux for biomass formation.

REDUCING THE COST OF EVALUATION OF THE GRADIENT AND THE HESSIAN OF MOLECULAR POTENTIAL ENERGY FUNCTIONS

C. Lavor[1] and N. Maculan[2]
[1]State University of Rio de Janeirom, Rio de Janeiro, RJ, Brazil
[2]Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil

One of the important points in molecular conformation problems [1] is the evaluation of the gradient and the Hessian of potential energy functions. These functions consist of a set of energy contributions, called the force field, for approximating the interactions beetwen atoms of a molecule. Our discussion will focus on potential energy functions that have common features of molecular force fields.

We can describe potential energy functions using Cartesian coordinates or internal coordinates (bond lengths, bond angles, and torsion angles). Analytic evaluation of the gradient with respect to the internal coordinates requires *O(n^4)* steps [2], whereas evaluating potential energy functions require *O(n^2)* steps (*n* is the number of atoms involved). Using the cosine law for torsion angles [3], we express potential energy functions in Cartesian coordinates and prove that the gradient and the Hessian are evaluated in *O(n^2)* and *O(n^3)* steps, respectively.

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GLOBAL OPTIMIZATION OF BIOPROCESSES USING STOCHASTIC AND HYBRID METHODS

J. R. Banga, C. G. Moles and A. A. Alonso
Process Engineering Group, IIM-CSIC, Spanish Council for Scientific Research
C/Eduardo Cabello 6, 36208 Vigo (SPAIN)

In this contribution, we will focus on problems arising in the context of biochemical process engineering. These problems can be stated as the optimization of non-linear dynamic systems. Examples of relevant problems in this domain are:

(a) optimal control problems (dynamic optimization)
(b) inverse problems (parameter estimation)
(c) simultaneous design and control optimization problems

Most of these problems are, or can be transformed to, nonlinear programming problems subject to differential-algebraic constraints. It should be noted that their highly constrained and non-linear nature often causes non-convexity, thus global optimization methods are needed to find suitable solutions.

Here, we will present our experiences regarding the use of several stochastic, deterministic and hybrid global optimization methods to solve those problems. Several parallel versions of the most promising methods, which are able to run on standard clusters of PCs, will also be presented.

Results for selected challenging case studies will be given. These cases include the optimal control of distributed diffusion-reaction systems, the simultaneous design and control of a wastewater treatment plant, and the robust estimation of kinetic parameters in complex reaction systems.

THE STEINER RATIO AND HOMOCHIRALITY OF BIOMACROMOLECULAR STRUCTURES

R. P. Mondaini and N. V. Oliveira

We report on the new improvement of the upper bound for the Steiner Ratio in 3-D Euclidean Space. The current value is given by

rho = (3*sqrt(3)+sqrt(7))/10
= 0.784190373377122...

and it was obtained by an assumption of regularity and periodicity of a special 3-D configuration. In this work we introduce another upper bound and the method used to derive it. We also give some ideas which relate the new value to the phenomenon of homochirality in the structure of biomacromolecules.

GLOBAL OPTIMIZATION UNDER NONLINEAR RESTRICTIONS BY USING STOCHASTIC PERTURBATIONS OF THE PROJECTED GRADIENT

J. E. Souza de Cursi [1] , R. Ellaia [2] , M. Bouhadi [2]
[1]Laboratoire de Mécanique de Rouen – UMR 6138 CNRS - Institut National des Sciences Appliquées de Rouen, Avenue de l'Université BP 08 - 76801 Saint Etienne du Rouvray CEDEX - France
[2]Laboratoire d'Etudes et Recherches en Mathématiques Appliquées – Université Mohammed V, Ecole Mohammadia d'Ingénieurs – BP 765, Agdal, Rabat - Morocco

Let us consider a regular (for instance, differentiable) function $J: R^n \rightarrow R$ and an admissible set $S \subset R^n$ given by

$$S = \{ x \in R^n \mid h_i(x) \leq 0 , \ i = 1, \ldots, m_i; \ h_i(x) \leq 0 , \ i = m_i + 1, \ldots, m \} ,$$

Where $h_i: R^n \rightarrow R$, $I = 1, \ldots, m$ are regular (for instance, twice continuously differentiable) functions. There is no convexity asumption on S and f. We denote by

$$x^* = \text{Arg Min } \{f(x) : x \in S\}$$

This problem can be numerically approximated by the projected gradient method introduced by Rosen., which is an iterative descent method generating a sequence $\{x_k\}_{k > 0}$ such that $x_{k+1} = Q(x_k)$. However, the convergence of such a method is ensured only if convexity asumptions are introduced ahich are not satisfied in the general situation above described.

In order to prevent convergence to local minima, stochastic perturbations of the descent method can be introduced by considering the modified descent method $x_{k+1} = Q(x_k) + P_k$, where P_k is a convenient random vector. The feasibility of such approach for linear restrictions is stated in the literature.

Here, the same approach is used in order to take into account nonlinear restrictions. A theorem of convergence is stated, analogous to the previously obtained for linear restrictions. We shall present numerical results.

ON GRADIENT FLOWS IN GLOBAL OPTIMIZATION

H. Th. Jongen
Aachen University, Germany
University Maastricht, The Netherlands

We consider finite dimensional differentiable optimization problems with a compact, connected feasible set. The focus will be on a basic problem in global optimization: how to get from one local minimum to all other ones using ascent or descent steps. The latter information will be provided by means of a Riemannian (i.e. variable) metric. We analyze a bang-bang strategy: starting at a local minimum, one goes upwards via the ascent flow until a local maximum is reached; then, via the descent flow one moves downwards to a (possibly other) minimum.

The latter idea gives rise to a directed bipartite graph whose nodes are the local minima/maxima. In absence of inequality constraints this digraph is connected for generic metrics. It turns out that the appearance of inequality constraints may cause stable obstructions for success. This is due to active set strategy. Nevertheless, (automatic) global adaptation of the metric involved may overcome the latter difficulty.

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GLOBAL OPTIMIZATION OF BILEVEL PROGRAMMING PROBLEMS VIA PARAMETRIC PROGRAMMING

E. N. Pistikopoulos, V. Dua, and J. Ryu
Centre for Process Systems Engineering, Imperial College London, UK

We present a global optimisation approach to the solution of bilevel linear and quadratic programming problems. The approach employs parametric programming principles for the solution of the inner problem, based on which the outer problem can be recast as a family of single (linear or quadratic) optimization problems, which can be solved to global optimality. Computational studies on several examples will be reported to highlight the key features of our proposed approach.

ALGORITHMS FOR QUADRATIC PROGRAMMING WITH SIMPLE BOUNDS

*Pasquale L. De Angelis[§], Paola Festa[&], and Gerardo Toraldo**
[§] Institute of Statistics and Mathematics, University Parthenope, Naples
[&]Dept. of Mathematics and Application
** Dept of Agricultural Engineering and Agronomy, University of Naples "FEDERICO II" , Italy*

Recently, a new heuristic for the global solution of box constrained quadratic problems, based on the classical results which hold for the minimization of quadratic problems with ellipsoidal constraints, has been presented [1]. In this work, for some special class of problems, such as the Maximum Clique problem, we discuss about some possible algorithmic modifications, that take into account of some new ideas recently proposed by the meta-heuristics research community. Further computational results are presented, that show some improvements with respect to the results in [1].

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ANALYSIS OF NON CONVEX POLYNOMIAL PROGRAMS BY THE METHOD OF MOMENTS

R. J. Meziat
Departamento de Matemáticas, Universidad de los Andes, Bogotá, Colombia

In this work we will propose a general procedure to estimate the global minima of mathematical programs given in the next general form

$$\begin{aligned} &\min \quad P_0(x) \\ &s.t. \qquad\qquad\qquad\qquad\qquad\qquad \textbf{(P)} \\ &P_i(x) \leq 0 \qquad for \quad i = 1, \dots, m \end{aligned}$$

where $P_0, \dots, P_m$ are n-dimensional polynomials which are not supposed to be convex. The theory behind the Method of Moments guarantees that all global minima of the non convex program (P) can be estimated by solving an equivalent convex program. One difficult question of the Method of Moments is how to characterize one particular convex set V of moment's vectors. In this work we solve the Multidimensional Truncated Moment's Problem in algebraic compact sets. Next we use this result for finding the global minima of non convex polynomial programs (P) by using an equivalent semidefinite program. In particular, we solve the general non convex quadratic program. Theory and several examples are explained in full detail.

A GLOBAL SMOOTHING ALGORITHM FOR GLOBAL OPTIMIZATION AND ITS APPLICATIONS

W. Murray
University Management Science and Engineering Stanford, California, USA

One of the most challenging optimization problems is determining the minimizer of a nonlinear programming problem in which there are some discrete variables. A particular vexing difficulty is the rate the work to solve such problems increases as the number of discrete variables increase. Any problem with discrete variables may be transformed to that of finding a {\em global} optimum of a problem in continuous variables. However, such transformed problems usually have astronomically large numbers of local minimizers, making them harder to solve than typical global optimization problems. Despite this apparent disadvantage, we show that the approach is not futile if we use smoothing techniques. The method we advocate first convexifies the problem and then solves a sequence of subproblems, whose solutions form a trajectory that leads to the required solution. To illustrate how well the new algorithm performs we show the computational results of applying it to some problems real world problems and also problems taken from the literature.

DETERMINISTIC GLOBAL OPTIMIZATION IN OPERATIONS RESAERCH

C. Y. Gau and L. Schrage*
**Lindo Systems*
University of Chicago, Chicago IL, USA

Attainment a guaranteed global optimum has been a long time goal in operations research. The desire for a global optimum occurs in decisions involving production planning, transportation, finance, inventory, resource allocation and more. Multi-starting/stochastic approaches are useful, but attaining a guaranteed best solution to a nonlinear/nonconvex model is obviously desirable.

We describe a deterministic global solver that searches until a global optimum is confirmed, rather than stopping after a first local optimum is found. The approach is based on converting the original nonlinear/non/smooth/ nonconvex model into several linear/convex subproblems, through use of a cutting-edge CIA (Convex, Interval and Algebraic) analysis. Then, a branch-and-bound technique is used to exhaustively search over these subproblems for the global solution. Once run to completion, it provides a mathematical guarantee to find the global optimum if any, or confirm the infeasibility if no solution exists.

Computational results will demonstrate the performance of the global solver for a wide variety of test problems from literatures as well as in real world applications. We discuss its capability in handling six categories of problems: continuous, mix-integer, logic-based disjunctive, complementarity, nonlinear equation solving, and probability/statistical estimation problems.

GLOBAL OPTIMIZATION TECHNIQUES FOR THE EIGENCOMPLEMENTARITY PROBLEM

Joaquim Judice[1], Isabel Ribeiro[2], and Hanif Sherali[3]
[1]University of Coimbra, Portugal
[2]University of Porto, Portugal
[3]Virginia Polytechnic Institute and State University, USA

Given a matrix $A ? R^{nxn}$ and a symmetric positive de_nite matrix $B ? R^{nxn}$, he Eigencomplementarity Problem, denoted by EICP, consists of _nding a positive real number $? ? R^1$ and a nonzero vector $x ? R^n$ such that

$(? B - A)x = 0; x = 0; (x; (? B - A)x) = 0$

where (,) denotes inner-product of two vectors. The EICP is shown to be NP-hard and finds applications in some contact problems in mechanics. The EICP is shown to be reduced to the problem of finding a stationary point of a quadratic function when A is symmetric. Other reformulations of the EICP as global optimization problems are dis-cussed for the general case together with some techniques for processing the corresponding problems. Some computational experience is included to highlight the efficiency of the global optimization techniques in this instance.

THE GENERALIZED αBB GLOBAL OPTIMIZATION APPROACH: TIGHT CONVEX UNDERESTIMATORS

I. G. Akrotirianakis and C. A. Floudas
Department of Chemical Engineering, Princeton University, Princeton, NJ, USA

In this paper we present an algorithm that locates the global optimum of nonconvex optimization problems that involve C2 functions. The algorithm is based on the principles of the deterministic global optimization algorithm αBB, and it also generates sequences of upper and lower bounds that converge to the global optimum. The novelty of the proposed approach is the way it constructs convex underestimators of arbitrarily nonconvex functions. The underestimators are derived by augmenting the original non-convex function by a nonlinear relaxation function. The relaxation function is a separable convex function, that involves the sum of univariate parametric exponential functions. An efficient procedure that finds the appropriate values for those parameters is developed. This procedure uses interval arithmetic extensively in order to verify whether the new underestimator is convex. For arbitrarily nonconvex functions it is shown that these underestimators are tighter than those generated by the αBB method. The role of the underestimating function is crucial to the performance of any deterministic algorithm. The tighter the underestimator the larger the lower bound is. Larger lower bounds help to fathom larger portions of the enumeration tree and thereby increase the performance of the overall algorithm. Extensive computational studies complemented with geometrical interpretations demonstrate the potential benefits of the proposed tight convex underestimators.

COMBINATORIAL AND CONTINUOUS APPROACHES TO THE MAX-CLIQUE PROBLEM

I. Bomze, M. Locatelli, and M. Pelillo
Institut fuer Statistik und Decision Support Systems, Universitaet Wien,
Dipartimento di Informatica,Università di Torino,
Dipartimento di Informatica, Università Ca' Foscari di Venezia

The Weighted Max-Clique Problem (WMCP) is a well known NP-hard problem even to approximate. In the recent paper [Massaro et al., 2002] a continuous approach to solve such problem has been proposed. The WMCP is reformulated as a Standard Quadratic Programming Problem (StQP), where the Hessian of the quadratic function is defined on the basis of the nodes' weights. Then, it is shown that from the local minima of such problem it is immediately possible to derive maximal cliques. Starting from this theoretical basis, the Pivoting Based Heuristic (PBH) has been proposed.
PBH is based on repeated applications of Lemke's method to detect KKT points of StQP as solutions of a Linear Complementarity Problem. In this talk we will first show that PBH turns out to be equivalent to a special Multistart greedy heuristic. Then, we will propose some modifications of such a heuristic in order to further increase the quality of the results with a limited amount of additional computation time. While the greedy approach always adds a node at each iteration, the first proposed modification introduces the possibility of swapping nodes, i.e. a node in the current clique is substituted by another one outside the current clique. In the second modification the greedy rule to select the next node to be added to the current clique is changed according to previously collected information. Such modifications have been tested over a selection of the DIMACS benchmarks showing a quite good improvement in the quality of the results with respect to the original greedy algorithm with a limited increase of the computational times.

ANALYTIC CENTERS CUTTING PLANE METHODS AND MIXED INTEGER PROGRAMMING, WITH EXTENSIONS TO SEMI-DEFINITE CUTS

J.-L. Goffin[1], S. Elhedhli[2], and M. R. Oskoorouchi[3]
[1]McGill University,Montreal, Quebec, H3A 1G5, Canada
[2]University W., Waterloo, On., Canada
[3]California State University San Marcos, San Marcos, California, USA

The most effective way to solve realistic MIPs (mixed integer programs) is branch and price, which is based on Lagrangean relaxation. Lagrangean relaxation provides better bounds than the traditional branch and bound method, which relax the integer requirement.

At every node of the B\&B tree, a nondifferentiable convex function (NDO) needs to be optimized. The classical NDO techniques, such as the Dantzig-Wolfe decomposition algorithm or subgradient optimization, have weaknesses, such as unreliable convergence or the lack of a rigorous termination criterion. The analytic center cutting plane method (ACCPM) attempts to improve over this.

We will sketch a full branch and price method that uses extensions of ACCPM, including Ryan and Foster branching and hot starts at the child nodes, using a dual Newton method.

Numerical results will be presented in problems arising in supply chain optimization.

Extensions of Dantzig-Wolfe column generation to semi-definite cuts will also be described, and numerical results in eigenvalue optimization will be reported. This can be used in a branch and sdp-cut framework. We also expect to report complexity results in the SOCP (Second order cone programming) cutting surface approach.

DISCRETE AND CONTINUOUS GLOBAL OPTIMIZATION IN OPERATIONS RESEARCH WITH THE VARIABLE NEIGHBORHOOD SEARCH METAHEURISTIC

N. Mladenovic
Mathematical Institute, Serbian Academy of Sciences and Arts, Yugoslavia

The basic idea of the recent metaheuristic known as Variable neighborhood search (VNS) is to allow a change of neighborhoods in the search for the better solutions. In this paper we first briefly give the rules of several VNS variants and then we discuss its applications in discrete and continuous optimization problems.

SOME CONNECTIONS BETWEEN DISCRETE AND CONTINUOUS OPTIMIZATION PROBLEMS

F. Tardella
University of Rome "La Sapienza", Rome, Italy

In the literature there are many examples of problems that have originally been formulated and solved as discrete or combinatorial optimization problems and that have subsequently been reformulated in a continuous setting in order to exploit complementary, and sometimes better, theoretical and computational results for their solution.
In a similar way, for many continuous optimization problems (with the most notable example of Linear Programming) it has been shown that the search for a global optimal solution can be restricted to a finite or discrete set of points thereby allowing for a discrete reformulation of the original problem.
One of the main tools used to establish the equivalence between discrete and continuous formulations of a minimization problem is some kind of concavity of the objective function.
We present here some general results that can be used to establish the equivalence between discrete and continuous optimization problems, we show that several equivalent formulations proposed in the literature can be easily established within our framework, and we propose some new discrete/continuous reformulation of continuous/discrete problems.

OPTIMIZATION PROBLEMS IN MASSIVE GRAPHS

P. M. Pardalos, V. Boginski, and S. Butenko
University of Florida, FL, USA

Massive data sets arise in a broad spectrum of scientific, engineering and commercial applications. These include finance, government and military systems, telecommunications, medicine and biotechnology, astrophysics, ecology, geographical information systems, etc [1]. Some of the wide range of problems associated with massive data sets are data warehousing, compression and visualization, information retrieval, clustering and pattern recognition, nearest neighbor search. Handling these problems requires special interdisciplinary efforts in developing novel sophisticated techniques. The pervasiveness and complexity of the problems brought by massive data sets make it one of the most challenging and exciting areas of research for years to come.

In many cases, a massive data set can be represented as a very large graph with certain attributes associated with its vertices and edges. These attributes may contain specific information characterizing a given application. Studying the structure of this graph is important for understanding the structural properties of the application it represents, as well as for improving storage organization and information retrieval. In this lecture we discuss recent advances in modeling and optimization for massive graphs. As examples, massive graphs arising in telecommunications, Internet, and finance will be used [2,3].

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EXACT PARALLEL ALGORITHM FOR COMPUTING MAXIMUM FEASIBLE SUBSYSTEMS OF LINEAR INEQUALITIES

Vera Rosta[1] *and Komei Fukuda*[2]
[1]*Department of Math/Stats, McGill University, Montreal QC, Canada*
[2]*School of Computer Science, McGill University, Montreal QC, Canada*

Given a system of linear inequalities, we consider the problem of finding a maximum feasible subsystem, that is a solution satisfying as many relations as possible. Amaldi and Kann point out that this general problem, called MAX FLS, is equivalent to the Closed Hemisphere Problem, which was shown to be NP-hard by Johnson and Preparata. To compute MAX FLS we consider the equivalent problem of finding the sign vector in a hyperplane arrangement with maximal number of nonnegative signs. We use a newly developed, hyperplane arrangement construction algorithm based on reverse search and linear programming which is memory efficient, highly parallelizable and output sensitive, i.e., polynomial in the size of input and output. A preliminary parallel implementation of the arrangement construction algorithm is available. This code can be adapted to solve the MAX FLS using our transformation and a bounding technique to eliminate unnecessary search. We also propose a similar hyperplane arrangement enumeration algorithm in computing multidimensional generalization of ranks in non-parametric statistic.

MINLP OPTIMIZATION FRAMEWORK USING SIMPLICIAL APPROXIMATION

M. Ierapetritou and V. Goyal
Rutgers - The State University of New Jersey, Piscataway, USA

An emphasis has been placed in recent years on the efficient solution of Mixed Integer Nonlinear Problems locally and globally. The need has been driven by the work of the mathematical programming community in the areas of process synthesis and design that has been significantly expanded recently in the areas of data mining, metabolic engineering and bioinformatics since most of the complex problems in these fields can be modeled as MINLP problems.

Existing local optimization approaches rely on convexity assumptions to determine the global optimum solution and the problem decomposition based on the ideas of projection, outer approximation and relaxation. For the cases of nonconvexities, existing global optimization frameworks are based mainly on branch and bound strategies and the use of underestimating functions to approximate the nonconvex constraints. Extensive reviews can be found in optimization textbooks by Floudas [1], [2].

In this paper we present a novel decomposition algorithm to solve MINLP problems. The approach guarantees the determination of the global optimum solution under the assumption that the objective function is convex and the set of equality and inequality constraints are convex, concave or quasi-concave functions and are continuous and once differentiable.

The proposed approach is based on the idea of closely approximating the feasible region defined by the set of constraints by a convex hull using the simplicial approximation approach. The simplicial approximation approach solves a series of line searches and NLP's to approximate the feasible region by a set of hyper-planes of its convex hull. The objective function is also linearized at the simplicial points.

For the case of concave and quasi-concave constraints the basic idea is the identification and approximation of the infeasible region where the process cannot operate. The infeasible region is then approximated from the outside using the outer polytope approach introduced in Goyal and Ierapetritou [3]. By eliminating the non-convexities the expanded feasible region is approximated using the simplicial approximation approach thus providing a complete representation of the feasibility region by a set of piece-wise linear hyper-planes. Using the linear approximations of the feasible region and objective function the proposed approach determines a valid lower bound to the optimum solution by solving a MILP problem. The binary variables are then fixed and a nonlinear problem is solved to determine a valid upper bound. Although close approximation of the optimum solution is achieved from the first iteration,

further improvement to a pre-specified tolerance can be obtained by refining the simplicial approximation of the feasible region. Theoretical convergence of the algorithm along with a number of computational examples are presented illustrating the applicability and efficiency of the proposed approach.

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GLOBAL OPTIMISATION FOR OIL RESERVOIR MODELLING

S. Gómez
IIMAS, National University of Mexico,
Longina Castellanos, ICIMAF, Academy of Science, Cuba
Nelson del Castillo, IIMAS, National University of Mexico

History Matching (parameter estimation) plays an important role in reservoir characterisation and monitoring. Due to the ill-posednes of this inverse problem, the least-squares optimisation has many local optima with good match, which produce alternative scenarios of production. These alternative solutions also provide a way to deal with the uncertainty of the modelling process.

Our aim is the generation of global optimisation methods that obtain many local optimal solutions with good match to the data in a stable way, and in reasonable computer time, to produce efficient decision making tools.
As the performance of the Tunnelling global method used in this work, depends on the local search methods used, we present here the results obtained when using a Truncated Gauss-Newton Method (TRON) and a Limited Memory Quasi-Newton Method (LBFGSB). The speed and robustness of the methods will be shown when tested on synthetic and real field cases

A new parallel version of the Tunneling methods and the improvement in the speed-up on a set of academic problems, including the molecular structure Lennard-Jones problem, will also be presented.

EXACT COMPUTATION OF GLOBAL MINIMA OF A NONCONVEX PORTFOLIO OPTIMIZATION PROBLEM

J. Kallrath
BASF-AG, GVC/S (Scientific Computing) Ludwigshafen, Germany
University of Florida, Astronomy Dept.,Gainesville, FL, USA

The goal of this project was to compute minimal cost solutions satisfying the demand of pre-given product portfolios and to investigate the dependence of the fix costs and investment costs on the product portfolio.

The most important parameters characterizing the production facilities are the number and the size of the reactors. The production is subject to shelf-life constraints, i.e., products cannot be stored longer than one week.

Even if we analyze this problem under the simple assumption of constant batch sizes and limit ourself to only one time period covering one week, the computation of minimum cost scenarios requires that we determine global minima of a nonconvex MINLP problem. A concave objective function and trilinear products terms involving the variables describing the number of batches, the utilization rates and the volume of the reactor are the nonlinear features in the model.

We have successfully applied three different solution techniques to solve this problem. (1) An exact transformation allows us to represent the nonlinear constraints by MILP constraints. Using piecewise linear approximations for the objective function the problem is solved with XPress-MP, a commercial MILP solver. (2) Convex underestimators coupled with a Branch-and-Bound scheme as implemented in aBB and SMIN-aBB. (3) The Branch-and-Reduce Optimization Navigator (BARON) called from the modeling system GAMS. In addition we applied the MINLP Branch-and-Bound solver SBB which is also part of GAMS.

GLOBAL RELIABILITY-BASED DESIGN OPTIMIZATION (THEORY AND APPLICATION)

G. Kharmanda[1], A. El –Hami[2] and N. Olhoff[3]
[1]Faculty of Mechanical Engineering, Aleppo University, Aleppo, Syria
[2]INSA de Rouen, LMR, 76801 St Etienne du Rouvray, France
[3]Institute of Mechanical Engineering, Aalborg University, Aalborg, Denmark

Two models are used in structural optimization: Deterministic Design Optimization (DDO) and Reliability-Based Design Optimization (RBDO). In the field of deterministic structural optimization, the designer reduces the structural cost without taking into account uncertainties concerning materials, geometry and loading. This way the resulting optimal design may represent a lower level of reliability and thus a higher risk of failure. Since structural problems are non-deterministic, it is clear that the introduction of the reliability concept plays an important role in the field of structural optimization. The integration of reliability analysis into the design optimization problem represents the RBDO model. The objective of this model is to design structures which should be both economic and reliable. The coupling between the mechanical mo deling, the reliability analyses and the optimization methods leads to very high computational cost and weak convergence stability. Since the traditional RBDO solution is achieved by alternating between reliability and optimization iterations, the structural designers performing deterministic optimization do not consider the RBDO model as a practical tool for the design of real structures. Fortunately, a hybrid method based on simultaneous solution of the reliability and the optimization problem has successfully reduced the computational time problem [KHA01]. The hybrid method allows us to satisfy a required reliability level, but the vector of variables here contains both deterministic and random variables. However, the hybrid RBDO problem is thus more comp lex than that of deterministic design. The major difficulty lies in the evaluation of the structural reliability, which is carried out by a special optimization procedure. Furthermore, both classical and hybrid RBDO may provide local optimal solutions. Here, the designer can obtain several local optima and then needs to select the best solution. Therefore, there is a strong motivation to develop a new technique that can overcome both drawbacks. In the present paper a new methodology based on the optimality conditions is proposed to provide the designer with the global optimal solution. This way we can compute the corresponding safety factors that satisfy a required reliability level without demanding additional computing cost for the reliability evaluation. The efficiency of this strategy is demonstrated on different examples [KHA02].

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GENERATOR OF CLASSES OF TEST FUNCTIONS FOR GLOBAL OPTIMIZATION ALGORITHMS

D. E. Kvasov[1], M. Gaviano, D. Lera[2], and Y. D. Sergeyev[3]
[1]University of Rome (Italy) and University of Nizhni Novgorod (Russia),
[2]University of Cagliari (Italy),
[3]University of Calabria (Italy) and University of Nizhni Novgorod (Russia),

Development of numerical algorithms for global optimization is strongly connected to the problem of construction of test functions for studying and verifying validity of these algorithms. Many of global optimization tests are taken from real-life applications and for this reason a complete information about them is not available. It often happens that there are not known a priori the number of local minima present in the problem, their locations, regions of attraction, and even values (including that one of the global minimum).

In this talk, a procedure for generating three types (non-differentiable, continuously differentiable, and twice continuously differentiable) of classes of test functions with known local and global minima for multiextremal multidimensional box-constrained global optimization is presented. The procedure consists of defining a convex quadratic function systematically distorted by polynomials in order to introduce local minima. Each test class provided by the generator consists of 100 functions constructed randomly and is defined by the following parameters: (i) problem dimension, (ii) number of local minima, (iii) value of the global minimum, (iv) radius of the attraction region of the global minimizer, (v) distance from the global minimizer to the vertex of the quadratic function. The other necessary parameters (i.e. locations of all minimizers, their regions of attraction, and values of minima) are chosen randomly by the generator. It is worthy to mention that multiple generation of a class with the same parameters produces the same 100 test functions. A special notebook with a complete description of all functions is supplied to the user. Partial derivatives are also generated where it is possible.

THE HINGE FITTING PROBLEM

M. Queiroz, C. Humes Jr., and J. Júdice
University of São Paulo, São Paulo, Brazil
University of Coimbra, Coimbra, Portugal

The Hinge Fitting problem is found in applications of neural networks, nonlinear regression and data classification. It consists in fitting n given points in $\Re^m$ by a hinge function, i.e. the maximum of two affine functions, as it appears in Breiman (IEEE Trans on Info Theory 1993; 39:999-1013) and Pucar & Sjöberg (IEEE Trans on Info Theory 1998; 44(3):1310-1318). This problem can be seen as a MPEC problem with a convex objective function.

For the euclidean error, an enumerative approach is proposed, which is shown to be a polynomial method in the sample size n, for a fixed dimension m. An alternative MPEC formulation for the l_1 error is also introduced, which is processed by a Sequential Linear Complementarity Problem approach.

Numerical results with both algorithms show that these methods compare favourably to previously proposed approaches.

A GENERAL FRAMEWORK FOR CONSTRUCTING COOPERATIVE GLOBAL OPTIMIZATION ALGORITHMS

X. Huang
AirPrism, Inc. Redwood Shores, CA, U.S.A.

Constraint-based optimization, which is NP-hard, describes a large class of problems in many fields, especially in formulating early perception tasks. In this paper, we first describe a new global optimization algorithm for attacking this problem. The algorithm divides a complex constraint-based optimization problem into a set of sub-problems of manageable complexities and search for the global optimal solutions following the principles of Cooperation, Coordination, and Compromising (CCC) as in the team playing. This algorithm is guaranteed to converge linearly, insensitive to the disturbances to its initial or intermediate solutions. It has the sufficient conditions to identify global solutions and the necessary conditions to trim the search spaces. Its power is demonstrated in solving nonlinear optimization problems raised from an early vision problem (shape from shading). Through 1,000 test problems, randomly generated by computer, the algorithm has a successful rate of 98.0% in finding the global solutions, while the conventional methods, Local Search and Simulated Annealing, have rates of 0.2% and 1.5%, respectively.

Most importantly in this paper, we propose a general framework for constructing the global optimization algorithms more powerful than the primary one. It is based on the partitions of the variable sets for breaking up problems and uses the lattice concept from the ABSTRACT #algebra to define the order of powers of the algorithms.

A MULTI-START METHODOLOGY FOR CONSTRAINED GLOBAL OPTIMIZATION USING NOVEL CONSTRAINED LOCAL OPTIMIZERS

J. A. Snyman, H. P. J. Bolton, and A. A. Groenwold
Department of Mechanical Engineering, University of Pretoria, Pretoria, South Africa

The constrained global optimization problem is addressed by using two relatively new constrained local optimization algorithms. The algorithms are the GLS1C [1] and the Dynamic-Q [2] algorithms, which both have relatively good global convergence capabilities. They are used in a multi-start strategy in combination with a Bayesian global stopping criterion [3]. The suitability of the stopping criterion is demonstrated for both the chosen local optimisation algorithms when used in multi-start mode and applied to standard test functions. The results show that for both algorithms the proposed methodology reliably and efficiently yields the global optimum of each problem. Particularly outstanding is the performance of the Dynamic-Q algorithm used in multi-start mode. Finally, parallelization of the sequential multi-start Dynamic-Q algorithm is shown to effectively reduce the computational expense associated with solving challenging global optimization problems.

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REPRESENTATION AND NUMERICAL DETERMINATION OF THE GLOBAL OPTIMIZER OF A CONTINUOUS FUNCTION ON A BOUNDED DOMAIN

J. E. Souza de Cursi
Laboratoire de Mécanique de Rouen, UMR 6138 CNRS – Institut National des Sciences Appliquées de Rouen – Avenue de l'Université BP 08 – 76801 Saint Etienne du Rouvray CEDEX - France

Let us consider $S \subset R^n$, closed, having a not empty interior, and $f: S \to R$ a continuous function. There is no convexity asumption on S and f. We denote by

$$x^* = \text{Arg Min } \{f(x) : x \in S\}$$

Let $\varepsilon > 0$ be a real number and $B^*(\varepsilon)$ the ball having center x^* and radius ε. We denote $S(\varepsilon) = S - B^*(\varepsilon)$. Let P be a probability on S and $g: R^2 \to R$ be a regular function such that $g \geq 0$. We denote by $\chi^*(\varepsilon,x)$ the characteristic function of $B^*(\varepsilon)$ and we assume that, for any $0 < \varepsilon < \varepsilon_0$:

- x^* is unique
- $P(B^*(\varepsilon)) > 0$
- $E(g(\lambda,f(x))) \geq h_1(\lambda,\varepsilon) > 0$;
- $E((1-\chi^*(\varepsilon,x)) g(\lambda,f(x))) = h_2(\lambda,\varepsilon)$,
- $h_2(\lambda,\varepsilon) / h_1(\lambda,\varepsilon) \to 0$ when $\lambda \to +\infty$

Then,

$$E(xg(\lambda,f(x)))/ E(g(\lambda,f(x))) \to x^* \text{ when } \lambda \to +\infty \ .$$

This result furnishes a representation of the global optimizer as the limit of a sequence of means. It generalizes a result of M. Pincus ans can be easily used in order to perform numerical evaluation of x^*.

We shall present numerical results using classical test functions of global optimization.

ADVANCES IN INTERVAL METHODS FOR DETERMINISTIC GLOBAL OPTIMIZATION IN CHEMICAL ENGINEERING

M. A. Stadtherr and Y. Lin
Department of Chemical Engineering, University of Notre Dame, Notre Dame, Indiana, USA

In recent years, it has been shown that strategies based on an interval-Newton approach can be used to reliably solve a variety of nonlinear equation solving and optimization problems in chemical process engineering, including problems in parameter estimation and in the computation of phase behavior. These strategies provide a mathematical and computational guarantee either that all solutions have been located in an equation solving problem or that the global optimum has been found in an optimization problem. The primary drawback to this approach is that computation time requirements may become quite high. In this presentation, we consider strategies for bounding the solution set of the linear interval equation system that must be solved in the context of the interval-Newton method. Recent preconditioning techniques for this purpose are reviewed, and a new bounding approach based on the use of linear programming (LP) techniques is presented. Using this approach it is possible to determine the desired bounds exactly (within round out), leading to significant overall improvements in computational efficiency. These techniques will be demonstrated using several global optimization problems, with focus on problems arising in chemical engineering, including parameter estimation and molecular modeling. These problems range in size from under ten variables to over two hundred, and are solved deterministically using the interval methodology.

EFFICIENT USE OF GRADIENT INFORMATION IN MULTIDIMENSIONAL INTERVAL GLOBAL OPTIMIZATION ALGORITHMS

L. G. Casado[1], J. A. Martínez[1], I. García[1], Y. D. Sergeyev[2] , and B. Tóth[3]
[1]Computer Architecture & Electronics Department., University of Almería, Sacramento SN, Almería. Spain.
[2]DEIS, Universita' della Calabria, Italy, and University of Nizhni Novgorod, Nizhni Novgorod, Russia.
[3]University of Szeged, Applied Informatics Department, Szeged, Hungary.

The performance of interval analysis branch-and-bound global optimization algorithms strongly depends on the efficiency of selection, bounding, elimination, division, and termination rules used in their implementation. All the information obtained during the search process has to be taken into account in order to increase algorithm efficiency, mainly when this information can be obtained and elaborated without additional cost (in comparison with traditional approaches). In this paper a new way to calculate interval analysis support functions for multiextremal and multidimensional functions is presented. The new support functions are based on obtaining the same kind of information used in interval analysis global optimization algorithms. The new support functions enable us to develop more powerful bounding, selection, and rejection criteria and, as a consequence, to significantly accelerate the search. Numerical results made on a wide set of multiextremal test functions are shown.

A NEW SUBINTERVAL SELECTION TECHNIQUE IN INTERVAL GLOBAL OPTIMIZATION

T. Csendes
University of Szeged, Hungary

The convergence properties of interval global optimization algorithms are studied that select the next subinterval to be subdivided with the largest value of the indicator pf(f_k,X). This time the more general case is investigated, when the global minimum value is unknown, and thus its estimation f_k in the iteration k has an important role. We present a new technique to ensure convergence to global minimizer points even for this case.

Extensive numerical tests will be completed on 40 problems to clear the positive efficiency impact of this new technique.

PROBABILITIES, INTERVALS, WHAT NEXT? OPTIMIZATION PROBLEMS RELATED TO EXTENSION OF EXTENSION OF INTERVAL COMPUTATIONS TO SITUATIONS WITH PARTIAL INFORMATION ABOUT PROBABILITIES

V. Kreinovich
University of Texas at El Paso, El Paso, Texas, USA

When we have only interval ranges [xi-,xi+] of sample values x1,...,xn, what is the interval [V-,V+] of possible values for the variance V of these values? We prove that the problem of computing the upper bound V+ is NP-hard. We provide a feasible (quadratic time) algorithm for computing the exact lower bound V- on the variance of interval data. We also provide feasible algorithms that computes V+ under reasonable easily verifiable conditions, in particular, in case interval uncertainty is introduced to maintain privacy in a statistical database.

We also extend the main formulas of interval arithmetic for different arithmetic operations x1 op x2 to the case when, for each input xi, in addition to the interval [xi]=[xi-,xi+] of possible values, we also know its mean Ei (or an interval [Ei] of possible values of the mean), and we want to find the corresponding bounds for y = x1 op x2 and its mean. In this case, we are interested not only in the bounds for y, but also in the bounds for the mean of y. We formulate and solve the corresponding optimization problems, and describe remaining open problems.

TERMINATION CRITERIA IN THE MOORE-SKELBOE ALGORITHM FOR GLOBAL OPTIMIZATION BY INTERVAL ARITHMETIC

M.H. van Emden and B. Moa.
Dept. of Computer Science, Victoria, B.C., Canada.

We investigate optimization with an objective function that has an unknown and possibly large number of local minima. The *fathoming* problem is the problem of determining *what* the global minimum is. The *localization* problem is the problem of determining *where* it occurs.

We adapt the Moore-Skelboe algorithm, and the way it uses interval arithmetic, to obtain versions specialized towards the fathoming problem and to obtain versions specialized towards the localization problem.

By using a suitable termination criterion, we obtain distinct versions that find the best lower bound and that find the best interval for the global minimum. In this way we address the fathoming problem.

The localization problem is important because often not only the global minimum is required, but also possibly existing points that achieve near-optimality. To support such a requirement, we define the *delta-minimizer*, the set of points at which the objective function is within delta of the global minimum. We obtain versions of the Moore-Skelboe algorithm that return a set of boxes that contain (are contained in) a delta-minimizer. Both version can be forced to return optimal results, taking into account the limitations imposed by the expression used to evaluate the objective function and the precision of the underlying arithmetic.

We prove theorems that show the correctness of the algorithms presented.

MATCHING STOCHASTIC ALGORITHM TO OBJECTIVE FUNCTION LANDSCAPE

W. P. Baritompa, M. Dur, E. M. T. Hendrix, M. Locatelli, L. Noakes, W. J. Pullan, and G. R. Wood

Department of Mathematics and Statistics, University of Canterbury, Christchuch, New Zealand
Department of Mathematics, Darmstadt University of Technology, Darmstadt, Germany
Group Operations Research and Logistics, Wageningen University, Wageningen, The Netherlands
Dipartimento di Informatica, Universitá di Torino, Torino, Italy
Department of Mathematics and Statistics, University of Western Australia, Perth, Australia
School of Information Technology, Griffith University, Gold Coast, Australia
Department of Statistics, Macquarie University, Sydney, Australia

Large scale optimisation problems are frequently solved using stochastic methods. Such methods often generate points randomly in a search region in a neighbourhood of the current point, backtrack to move past barriers and employ a local optimiser. The aim of this presentation is to explore how these algorithmic components should be used, given a particular objective function landscape. In a nutshell, we begin to provide rules for efficient travel, if we have some knowledge of the large or small scale geometry.

STOCHASTIC ADAPTIVE SEARCH METHODS BASED ON HIT-AND-RUN SAMPLING FOR DISCRETE AND CONTINUOUS GLOBAL OPTIMIZATION

Z. B. Zabinsky and Y. Shen
Industrial Engineering Program, University of Washington, Seattle, WA USA

Hit-and-Run has been used as a generator for simulated annealing type algorithms for continuous global optimization, motivated by theoretical analysis of adaptive search. When temperature is zero, Improving Hit-and-Run has $O(n^{5/2})$ function evaluations on a class of elliptical programs. An analogous development for discrete global optimization is explored. First, a Discrete Hit-and-Run (DHR) Markov chain sampler is used, that converges to an arbitrary discrete distribution over a bounded subset of an n-dimensional integer lattice. It converges to a uniform distribution on an n-dimensional hyperrectangle integer lattice in $O(n^3)$. Several versions of DHR are discussed. One version is shown to converge to Hit-and-Run as the discrete mesh becomes finer and approaches a continuous space.

An attempt to implement discretized adaptive search using a simulated annealing approach with DHR generator is presented. The addition of a temperature parameter changes the underlying distribution to Boltzmann, which is also discussed. Improving Discrete Hit-and-Run algorithm (with temperature zero), based on the theoretical analysis of pure adaptive search on a finite discrete space is introduced, and computational results using several versions of the underlying sampler are presented.

OPTIMIZING THE GLOBAL RANDOM SEARCH METHODS BASED ON STATISTICAL INFERENCE ABOUT THE OBJECTIVE FUNCTION

A. Zhigljavsky and A. Zilinskas
Cardiff University, UK

The so-called branch and probability bound methods are global random search methods based on the use of statistical inference about the maximum value of the objective function in different subsets of the feasible domain.
The statistical inference are made on the base of the asymptotic theory of order statistics obtained from a random or semi-random sample of points in the regions that are tested for prospectiveness for further search. In the present work, we derive asymptotic expressions for the length of the confidence regions for the maximum values and on the base of these asymptotic expressions we optimize (for certain classes of the objective functions) the parameters of the global optimization algorithms.

A ONE DIMENSIONAL GLOBAL OPTIMIZATION ALGORITHM FOR OBSERVATIONS WITH NOISE

A. Zilinskas[1] and J. M. Calvin[2]
[1]IMI, Vilnius, Lithuania, and Cardiff University, UK
[2]New Jersey Institute of Technology, USA

The problem of global optimization of multimodal functions in the presence of noise is one of the most difficult in optimisation theory. An approach to global optimization based on statistical models of the objective function is well-suited for incorporation of function evaluations with random noise. In this talk we describe a global optimization algorithm for continuous univariate functions in the case where function evaluations are corrupted by independent Gaussian noise. The approach is based on modeling the objective function as a Wiener process.

We derive the conditional distributions, which are also Gaussian. The standard formulae (involving inversion of covariance matrix) are reduced to a recurrent algorithm. Further simplification is achieved by means of truncation of the recurrence. The proposed simplifications imply a dramatic reduction in complexity of the adaptive optimisation algorithms, for example the P-algorithm. We investigate the theoretical convergence rates attainable with nonadaptive and adaptive methods for choosing the observation points. The theoretical results are compared with the results of numerical testing.

GLOBAL OPTIMIZATION OF HOMOGENEOUS FORMS

L. Faybusovich
Department of Mathematics, University of Notre Dame, USA

We consider new semidefinite and linear programming approximations for Problems of optimization of a homogeneous form on the sphere and the simplex. Unlike previous results exact estimates are provided for the accuracy of these approximations. The results generalize previous work of Nesterov, DeKlerk and others where the case of a quadratic form hs been considered

AN INTERIOR POINT HEURISTIC FOR THE HAMILTONIAN CYCLE PROBLEM VIA MARKOV DECISION PROCESSES

V. Ejov[1], J. A. Filar[1], and J. Gondzio[2]
[1]School of Mathematics, University of South Australia, Australia
[2]Dept. of Maths and Stats, University of Edinburgh, Scotland, UK

We consider the Hamiltonian cycle problem embedded in a singularly perturbed Markov decision process (MDP). More specifically, we consider the HCP as an optimization problem over the space of long-run state-action frequencies induced by the MDP's stationary policies. We show that Hamiltonian cycles (if any) correspond to the global minima of a suitably constructed indefinite quadratic programming problem over the above frequency space. We develop an interior-point type algorithm that involves an arc elimination heuristic that appears to perform rather well in moderate size graphs. The approach has the potential for further heuristic developments.

ON A CLASS OF QUASI-HEMIVARIATIONAL INEQUALITIES

Z. Naniewicz
Cardinal Stefan Wyszynski University, Faculty of Mathematics and Science, Warsaw, Poland

A class of quasi-hemivariational inequality on a vector valued function space is studied. We are to deal with a system of hemivariational inequalities involving Clarke partial derivatives. Namely, the problem is to find $u \in V \subset W^{1,p}(\Omega; R^N), p > 1$ such as to satisfy the inequality:

$$\langle Au - g, v - u \rangle_V + \int_\Omega \sum_{k=1}^{N} f^0_{(k)}(u; v_k - u_k) d\Omega \geq 0, \quad \forall v \in V,$$

where $f^0_{(k)}(\cdot;\cdot)$ is a directional Clarke derivative in the k-th direction. The higher order term expressed by A is assumed to be monotone and coercive. The approach relies on nonsmooth variational methods using essentially a general unilateral growth condition of the form

$$f^0_{(k)}(x, \xi; -\xi_k) \leq \alpha_k (1 + |\xi|^q), \quad \forall \xi \in R^N, \quad k \in \{1, ..., N\},$$

and a new concept of solution. This notion of solution reduces to the usual concept when further regularity is available. The weak growth hypothesis makes impossible to curry out within the framework of reflexive Banach spaces only. The scheme of our reasoning is to deal with a Galerkin basis of V, solve the corresponding finite dimensional problems and then pass to the limit by making use of some compactness arguments involving Dunford Pettis criterion.
Some applications to nonmonotone variational problems of mechanics are given.

QUASICONVEXITY, FRACTIONAL PROGRAMMING AND EXTREMAL TRAFFIC CONGESTION

C. E. M. Pearce
Department of Applied Mathematics, University of Adelaide, Australia

A classical problem in telecommunications is the determination of the extremal time congestion that can arise in a GI/M/N/N loss system with given arrival and service rates. A central difficulty was showing that a local extremum has to be global. The matter stood unresolved for many years but has recently been settled using quite delicate convex analysis. We treat this problem and some generalisations in a simpler way by making use of quasiconvexity.

GLOBAL SOLUTION OF OPTIMIZATION PROBLEMS WITH DYNAMIC SYSTEMS EMBEDDED

P. I. Barton and A. B. Singer
Massachusetts Institute of Technolog, Cambridge, Massachusetts, USA

This paper develops deterministic global optimization algorithms for problems involving nonconvex objective and constraint functionals with dynamic systems embedded. Algorithms for both linear and nonlinear embedded dynamics are developed. The techniques utilized for each problem classification are unified by an underlying composition principle that transfers any nonconvexity in the embedded dynamics into the objective and constraint functionals. By generating a pointwise in time convex relaxation for an integrand, convex relaxations for integral functionals are derived. These convex relaxations are then utilized in either a spatial branch-and-bound algorithm to determine the global minimum of a dynamic optimization problem or in a nonconvex outer approximation algorithm for mixed-integer dynamic optimization.

For problems with linear dynamics embedded, we show that the solution to the state equations is affine in the decision variables. The affine solution is combined with derived exact state bounds and a standard convexity lemma to yield the convex composition result. For the nonlinear case, McCormick's composition result is applied recursively to generate a convex underestimator for the integrand. The requisite convex and concave bounding functions are supplied by a novel method for deriving linear bounding systems for the right hand sides of general nonlinear ordinary differential equation systems. Upon integration, these linear dynamic systems yield convex underestimators and concave overestimators valid over the decision variable space for each fixed time. Numerical results for both the linear and nonlinear cases will be presented.

A DETERMINISTIC GLOBAL OPTIMIZATION ALGORITHM FOR PROBLEMS WITH NONLINEAR DYNAMICS

C. S. Adjiman and I. Papamichail
Imperial College of Science, Technology & Medicine, London, UK

A deterministic spatial branch and bound global optimization algorithm is presented for systems with an initial value problem for a set of first-order, typically nonlinear, differential equations in the constraints. Upper bounds on the global minimum are obtained using the sequential approach for the local solution of the dynamic optimization problem. The solution of a convex relaxation of the problem provides lower bounds. Well-known convex underestimation techniques are used for the relaxation of the algebraic functions. The concept of differential inequalities is uaegetilized for the development of parameter independent as well as parameter dependent bounds on the dynamic system. Three new convex relaxation procedures are proposed for the parameter dependent solution of the initial value problem. The global optimization algorithm is illustrated by applying it to several case studies relevant to chemical engineering.

NEW RESULTS IN DETERMINISTIC GLOBAL OPTIMIZATION FOR PROBLEMS WITH ORDINARY DIFFERENTIAL EQUATIONS

B. Chachuat and M. A. Latifi[*]
Laboratoire des Sciences du Génie Chimique, UPR 6811, CNRS-ENSIC,
1 rue Grandville, BP 451, 54001 Nancy Cedex, France

Optimization problems with ordinary differential equations are common in chemical engineering and many other engineering fields. Typical examples are the determination of optimal operating profiles for batch and semi-continuous processes, or the parameter estimation of differential systems from experimental data. The classical methods used to solve these problems are based either on variational methods or on discretization approaches to yield finite dimensional optimization problems. However, both are local optimization methods and result in suboptimal solutions if the problems exhibit nonconvexities. This is rather true for the dynamic optimization problems encountered in chemical engineering applications and the use of suboptimal solutions can have a significant impact from the economical, environmental or safety points of view. In order to overcome the convergence to local minima, stochastic as well as deterministic global optimization methods may be applied. Only deterministic methods, *i.e.* methods which can guarantee locating the global solution in a finite number of iterations, are considered in the sequel.

Several recent deterministic global optimization methods have been derived for dynamic problems. Singer and Barton [7] developed methods to solve linear dynamic systems embedded optimization problems. Smith and Pantelides [8] performed complete discretization and symbolic manipulations, and then applied the spatial branch-and-bound algorithm; similarly, Esposito and Floudas [4] used the complete discretization approach and applied the αBB algorithm [2, 1] in order to solve parameter estimation problems. However, these methods were found to perform poorly, sometimes even failing to achieve convergence. Building upon the αBB framework, a rigorous algorithm was also derived from the use of control parameterization [3], and a method was further proposed to compute rigorous convex underestimators for differential constraints from the concept of differential inequalities [6].

In this contribution, an alternative approach to build convex relations of dynamic problems is proposed. It is demonstrated that a nonconvex state-dependent functional F of the following form:

$$F(p) = g\left(x(t_f), p\right) + \int_{t_0}^{t_f} L(x(t), p, t)dt$$

$$\text{with :} \quad \dot{x}(t) = f(x(t), p), \forall t \in [t_0, t_f]$$

$$x(t_0) = h(p)$$

with $p \in \mathbb{R}^{n_p}$ and $x \in \mathbb{R}^{n_x}$ being the parameter and the state vectors respectively, p^L and p^U being the bounds on the parameters, and f, L, f and h being twice-differentiable maps, can be underestimated by directly adding a quadratic term as:

$$\breve{F}(p) = F(p) + \sum_{k=1}^{n_p} \alpha_k \left(p_k^U - p_k\right)\left(p_k^L - p_k\right)$$

In addition, a method was developed to compute values of the α's which guarantee that $\breve{F}$ is a rigorous convex underestimator of F, based on interval analysis, the concept of differential inequalities and the convexity theory. It is also anticipated that the method could be extended to index 1 differential-algebraic systems embedded.

A global optimization algorithm for dynamic problems is obtained by applying this convex relaxation method within a branch-and-bound framework (similarly to the αBB algorithm) and using the optimization software DYNO [5]. Applications to chemical engineering problems are currently under investigation.

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GLOBAL DYNAMIC OPTIMIZATION OF LINEAR HYBRID SYSTEMS

C. Kun Lee and P. I. Barton
Department of Chemical Engineering, Massachusetts Institute of Technology, USA

Hybrid systems, which exhibit both discrete state and continuous state behavior, have become the modeling framework of choice for a wide variety of applications that require detailed dynamic models with embedded discontinuities. Economic, environmental, safety and quality considerations in these applications, such as the automated design of safe operating procedures and the formal verification of embedded systems, strongly motivate the development of algorithms and tools for the global optimization of hybrid systems. For safety critical tasks such as formal verification, it is crucial that the global solution be found within epsilon optimality.

Recently, a deterministic algorithm has been proposed for the global optimization of linear time varying hybrid systems in the continuous time domain, provided the transition times and the sequence of modes are fixed. This work is extended by presenting a method for determining the optimal mode sequence when the transition times are fixed. A reformulation of the problem by introducing binary decision variables while retaining the linearity of the underlying dynamic system is proposed. This allows recently developed convexity theory for linear time varying continuous systems to be employed to construct a convex relaxation of the resulting mixed-integer dynamic optimization problem, which enables the global solution to be found in a finite number of iterations using nonconvex outer approximation.

SUBMISSION TO 4TH INTERNATIONAL CONFERENCE ON FRONTIERS IN GLOBAL OPTIMIZATION ROUTING IN OPTICAL AND CIRCUIT-SWITCHED NETWORKS

A. E. Ozdaglar and D. P. Bertsekas
Massachusetts Institute of Technology, Cambridge, Massachusetts, USA

The problem of routing and wavelength assignment (RWA) is critically important for increasing the efficiency of wavelength-routed all-optical networks. Given the physical network structure and the required connections, the RWA problem is to select a suitable path and wavelength among the many possible choices for each connection so that no wo paths sharing a link are assigned the same wavelength. In work to date, this problem has been formulated as a difficult integer programming problem that does not lend itself to efficient solution or insightful analysis. In this work, we propose several novel optimization approaches that offer the promise of radical improvements over the existing methods. We propose new integer-linear programming formulations, which can be addressed with highly efficient linear (not integer) programming methods and yield optimal or near-optimal RWA policies. The fact that this is possible is surprising, and is the starting point for new and greatly improved methods for RWA. The methodology applies as a special case to the problem of routing in circuit-switched (nonoptical) networks.

THE USE OF GLOBAL OPTIMIZATION IN THE STUDY OF DATA FUSION

F. Zirilli
Dipartimento di Matematica G. Castelnuovo, Università di Roma La Sapienza, Italy

We consider the problem of data fusion. That is: given a "scene" (i.e. for example a piece of the Earth surface or a piece of the human body) observed with several sensors (i.e. for example radars, optical instruments or CT-Computerized Tomography, MRI-Magnetic Resonance Imaging), we want to exploit the redundancy of information coming from the presence of several sensors observing the same scene when interpreting the data.
Note that data fusion is already an active research area in engineering and is becoming an important subject in the emerging field of image science in applied mathematics.
We will provide several formulations of the data fusion problem as a global optimization problem. These mathematical models are based on simple ideas taken from calculus of variations and provide a mathematical setting to consider several problems in signal processing such as filtering, segmentation and classification of images.
The global optimization problems coming from data fusion are usually formulated in high dimension and are ill conditioned. With this in mind we discuss some numerical algorithms to solve them.
Finally we present an application to the data fusion problem coming from the use of SAR (Synthetic Aperture Radar) and optical data of a portion of the Charles de Gaulle airport in Paris (France).
The work presented is a development of the work shown in:
http://www.web.unicam.it/matinf/fatone/esrin.asp
http://www.web.unicam.it/matinf/fatone/w1

AN EFFICIENT ALGORITHM FOR THE MINKOWSKI ADDITION OF CONVEX POLYTOPES

K. Fukuda
School of Computer Science, McGill University, 3480 University Street, McConnell Engineering Building, Montreal, Canada

A zonotope is the Minkowski addition of line segments in R^d. The zonotope construction problem is to list all extreme points of a zonotope given by k line segments. By duality, it is equivalent to the arrangement construction problem that is to generate all regions of an arrangement of k hyperplanes in R^d

By replacing line segments with convex V-polytopes, we obtain a natural generalization of the zonotope construction problem: the construction of the Minkowski addition of k polytopes. Gritzmann and Sturmfels studied this general problem in various aspects and presented polynomial algorithms for the problem when one of the parameters k or d is fixed.

The main objective of the present work is to present an efficient algorithm for variable d and k. Here we call an algorithm efficient or polynomial if it runs in time bounded by a polynomial function of both the input size and the output size. The algorithm is a natural extension of a known algorithm for the zonotope construction, based on linear programming and reverse search. It is compact, highly parallelizable and very easy to implement.

This work has been motivated by the use of polyhedral computation for optimal tolerance determination in mechanical engineering. Other applications have been reported in computational algebra, automatic control theory.

EFFECTIVE LOCAL SEARCH ALGORITHMS FOR THE VEHICLE ROUTING PROBLEM WITH GENERAL TIME WINDOW CONSTRAINTS

T. Ibaraki[1], S. Imahori[1], M. Kubo[2], T. Masuda[3], T. Uno[4] and M. Yagiura[1]
[1]Kyoto University
[2]Tokyo University of Mercantile Marine
[3]Accenture Inc.
[4]National Institute of Informatics

Abstract: We propose local search algorithms for the vehicle routing problem with soft time window constraints. The time window constraint for each customer is treated as a penalty function, which is very general in the sense that it can be non-convex and discontinuous as long as it is piecewise linear. The generality of time window constraints allows us to handle a wide variety of scheduling problems. In our algorithm, we use local search to assign customers to vehicles and to find orders of customers for vehicles to visit. It employs a new neighborhood, called the cyclic exchange neighborhood, in addition to standard neighborhoods for the vehicle routing problem. After fixing the order of customers for a vehicle to visit, we must determine the optimal start times of processing at customers so that the total penalty is minimized. We solve this non-convex problem by using dynamic programming, and employ sophisticated data structures to make it efficient. We also report computational results for various benchmark instances of the vehicle routing problem, as well as real world instances of a production scheduling problem.

APPLYING GLOBAL OPTIMIZATION TO ENHANCE GRAPH THEORY: THE AUTOGRAPHIX 1 AND AUTOGRAPHIX 2 SYSTEMS

G. Caporossi and P. Hansen
GERAD and HEC Montreal, CANADA

Computers are extensively used in graph theory to find values of invariants, such as chromatic number, independence number, diameter, radius and the like, to enumerate graphs of various families and to assist in proofs, also by enumeration. They can also be used to enhance graph theory *per se* by

(i)finding extremal graphs for some invariants or formula involving several invariants,
(ii)finding such extremal graphs subject to constraints,
(iii)refuting conjectures and/or strengthening them,
(iv)finding original conjectures and
(v)suggesting proof strategies.

The AutoGraphiX 1 and AutoGraphiX 2 systems use global optimization for the purposes listed above: extremal or near-extremal graphs are first obtained with the Variable Neighborhood Search metaheuristic; then three methods, numerical, algebraic and geometric, are applied to find conjectures automatically. This has led to over 60 conjectures and a dozen research papers.

The AutoGraphiX 2 system will be described, with a focus on the global optimization routines which are at its heart. Several original conjectures will also be presented.

EXACT AND HEURISTIC APPROACHES FOR A CYCLIC DELIVERY PROBLEM.

P. Festa[1] and R. Cerulli[2]
[1]DMA, Università degli Studi di Napoli FEDERICO II, Italy.
[2]DMI, Università degli Studi di Salerno, Italy.

In this paper, a scheduling problem for pseudo-cyclic deliveries is considered, in which each user in prefixed time periods requires a given amount of commodity, subject to the constraints that two successive deliveries (of commodity) must be spaced by an exact given number of instants. The objective function is the minimization of the centralized supplier capacity needed to satisfy the user requests over a discretized planning horizon. It is easy to prove the NP-hardness of the problem. We propose two pairs of algorithms, each made by a Branch and Bound (B&B) procedure for exactly solving small instances and a greedy heuristic algorithm for facing real world sized instances. The algorithms of the first pair are a classical B&B and a very easy greedy heuristic approach that do not fully exploit any characteristic of the problem. Instead, the second pair solves more efficiently the problem, taking into account some important properties of its structure, such as decomposition principle.
For showing the effectiveness of the enhanced heuristic approach of the second pair of algorithms we compare the obtained solutions either to the exact solutions provided by the B&B algorithm or to lower bounds.

A RELIABLE COMPUTER METHOD FOR THE ``PACKING CIRCLES IN A UNIT SQUARE'' PROBLEMS

M. C. Markot and T. Csendes
University of Szeged, Hungary

We are dealing with the problem of finding the densest packings of non-overlapping equal circles within a square. In order to provide reliable numerical results, the developed algorithm is based on interval analysis. As one of the most efficient parts of the algorithm, an interval based version of a previous elimination procedure is introduced. This method represents the remaining areas still of interest as polygons fully evaluated in interval way. Currently the most promising way of finding optimal circle packing configurations is the partitioning of the original problem into subproblems. Still as a result of the highly increasing number of subproblems, earlier computer-aided methods were not able to solve problem instances where the number of circles was greater than 27.
The present paper provides a carefully developed technique resolving this difficulty by eliminating large groups of subproblems.

As a demonstration of the capabilities of the new algorithm, the problems of packing 28, 29, 30 circles are solved with mathematical rigour. Our results confirm the optimality of the earlier found solutions within a very tight tolerance value.

A DECOMPOSITION-BASED ALGORITHM TO THE WATER IRRIGATION NETWORK DESIGN PROBLEM

G. M. Gonçalves [1], and M. V. Pato[2]
[1]Department of Mathematics, Faculty of Sciences and Technology, New University of Lisbon, Portugal
[2]Department of Mathematics, Faculty of Economics and Business Administration, Technical University of Lisbon, Portugal

The authors consider the problem of designing a water distribution network to feed a pressurized irrigation system. The process of designing such a network has been historically subdivided into three phases: firstly selection of the network topology, secondly evaluation of the flows to be conveyed by the network arcs, and finally, dimensioning of the network's hydraulic components – consisting of the pipes and the pumps – besides assignment of the pump facilities. In this presentation the authors propose a mixed-binary nonlinear programming model for the overall problem and discuss an alternative solution approach. The model is non-convex and its nonlinear and non-convex nature arises from nonlinear relations in the continuous domain only. By fixing some continuous variables the model becomes convex and this is used to develop a decomposition-based algorithm. The paper concludes with a display of computational results.

A FUZZY PARTITIONING BASED PRE-SCREENING METHOD FOR IMPROVED SEARCH EFFICIENCY IN GLOBAL OPTIMIZATION

L. Ozdamar[1], M. Basak Demirhan[2], and E. Onbasioglu[3],
[1]Nanyang Technological University, Faculty of Mechanical and Production Eng., Systems and Engineering Management Division, Singapore
[2]Yeditepe University, Dept. of Systems Engineering, Istanbul, Turkey
[3]Yeditepe University, Dept. of Computer Engineering, Istanbul, Turkey

This work describes a fuzzy information retrieval and partitioning method that aims to identify sub-spaces that are not likely to contain the extremities of a function. The method produces a topology where regions unlikely to contain extremities are deducted from the feasible space and the complementary area is reported for further investigation. The approach of building up topologies from a limited set of discrete data stems from the field of visualization and image re-construction. Here, an efficient information retrieval methodology is developed to fully exploit a given set of available data before a full-scale search is applied to identify the global optima. The approach integrates fuzzy assessment and fuzzy partitioning that work together to obtain a reliable classification of the feasible space. The method provides a good pre-screening tool for stochastic search techniques and reduces the number of function evaluations required to locate extremities. Its practical value becomes more significant when the function is unknown, or when it is expensive to evaluate the function. Numerical results on test functions with various difficulty levels (obtained from the literature) show that the proposed method achieves its goal.

2003 & Upcoming Aegean Conferences

2nd Workshop on Complement Associated Diseases, Animal Models, and Therapeutics
June 1-6, 2003 | Myconos, Greece

4th International Conference on Frontiers in Global Optimization
June 8-12, 2003 | Santorini, Greece

Pathways, Networks, and Systems: Theory and Experiments
September 28 - October 2, 2003 | Santorini, Greece

Autoimmunity: Mechanisms and Novel Treatments
Endorsed by CIS/FOCIS
October 8-13, 2003 | Myconos, Greece

Symposium on Tissue Engineering Science
October 3-8, 2004 | Crete, Greece

3rd Lymphocyte Signal Transduction Workshop
May 31 - June 4, 2004 | Myconos, Greece

3rd Innate Immunity Workshop
June 7-11, 2004 | Crete, Greece

2nd Gene Regulation in Lymphocyte Development
May 23-28, 2005 | Myconos, Greece

3nd Workshop on Complement Associated Diseases, Animal Models, and Therapeutics
October 9-15, 2005 | Crete, Greece

The Philosophy of Science
October 16-21, 2005 | Crete, Greece