Advances in Global Optimization: Methods and Applications

Myconos, Greece – June 13-17, 2007

Organizers: **Christodoulos A. Floudas (floudas@titan.princeton.edu)**
Panos M. Pardalos (pardalos@ufl.edu)

Reception: **Tuesday, June 12th at 8:00 pm**

Gala dinner: **Saturday, June 16th at 8:00 pm**

Conference Program

Wednesday, 13th June

	7:00	8:15	Registration
	8:15	8:25	P.M. Pardalos and C.A. Floudas Welcome from the Organizers
1	8:25	8:50	Benjamin Ivorra (speaker), Bijan Mohammadi and Ángel Manuel Ramos del Olmo A Semi-Deterministic Global Optimization Method for Credit Portfolio Optimization under Constraints
2	8:50	9:15	Dietmar Maringer and Panos Parpas (speaker) Global Optimization of Higher Order Moments in Portfolio Selection
3	9:15:	9:40	Balazs Banhelyi and Tibor Csendes (speaker) Global Optimization in Computer-Assisted Proofs
4	9:40	10:05	Massimiliano Vasile, Nicolas Croisard (speaker) Reliable Trajectory Design Through Evidence Theory and Multiobjective Optimisation
5	10:05	10:30	Panos Parpas (speaker), Efstratios Pistikopoulos and Berc Rustem Global Optimization of Robust Chance Constraint Problems
	10:30	11:00	Coffee Break
6	11:00	11:25	E. Davis and Marianthi G. Ierapetritou (speaker) A New Method of Addressing Process Synthesis Containing Black-Box Functions
7	11:25	11:50	Hanif D. Sherali (speaker) and Jitamitra Desai Global Optimization Models and Algorithms for the Management of Cascading Risks via Event Trees
8	11:50	12:15	Massimiliano Vasile, Matteo Ceriotti (speaker) and Paolo De Pascale An Incremental Approach to the Solution of Global Trajectory Optimisation Problems
9	12:15	12:40	Josef Kallrath (speaker) Packing Circles and Convex Polygons into Area-Minimizing Rectangles
10	12:40	13:05	Josef Kallrath, Steffen Rebennack (speaker) and Panos M. Pardalos Column Enumeration based Decomposition Techniques for a Class of Non-Convex MINLP Problems
11	13:05	13:30	Tapio Westerlund (speaker) Some Transformation Techniques with Applications in Global Optimization

Thursday, 14th June

1	15:00	15:25	Angelo Lucia (speaker) and Rajeswar R. Gattupalli A Multi-Scale Approach to Global Optimization for Molecular Conformation Problems
2	15:25	15:50	P. Foteinou, M.G. Ierapetritou and I.P. Androulakis (speaker) Global Optimization Approaches for the Synthesis of Regulatory Networks
3	15:50	16:15	Yin Zhang (speaker) A New Approach to Fluence Map Optimization in IMRT
4	16:15	16:40	K.M. Rajesh (speaker) and Asim K. Pal A Note on Funnel Functions
5	16:40	17:05	Monica Cojocaru (speaker) Vaccination Strategies Dynamics of Population Groups with Distinct Perceived Probabilities of Infection
6	17:05	17:30	Graham Wood (speaker) Finding Optimal Feeding Schedules in Pig Production
7	17:30	17:55	Orcun Molvalioglu, Zelda B. Zabinsky (speaker) and Wolf Kohn The Interacting-Particle Algorithm with Dynamic Heating and Cooling

Friday, 15th June

1	8:00	8:25	C.E. Gounaris and C.A. Floudas (speaker) Tight Convex Underestimators for C^2-Continuous Problems
2	8:25	8:50	R.P. Mondaini (speaker) An Analytical Method for derivation of the Steiner Ratio of 3D Euclidean Steiner Trees
3	8:50	9:15	Jürgen Garloff and Andrew P. Smith (speaker) Fast and Tight Polynomial Bounds Based on Bernstein Expansion
4	9:15	9:40	Hubertus Th. Jongen (speaker) On the Min-Max Graph in Finite and Semi-Infinite Optimization
5	9:40	10:05	Fabio Tardella (speaker) Existence and construction of polyhedral convex envelopes
6	10:05	10:30	Laura Di Giacomo (speaker) An Interior Point Newton Method for General Bounded Linear Complementarity Problems
	10:30	11:00	Coffee Break
7	11:00	11:25	Antanas Žilinskas and Julius Žilinskas (speaker) Branch and Bound Algorithm for Multidimensional Scaling with City Block Metric
8	11:25	11:50	Le Hoai Minh, Le Thi Hoai An (speaker), Pham Dinh Tao and Bouvry Pascal A Combined DCA - GA for Constructing Highly Nonlinear Balanced Boolean Functions in Cryptography
9	11:50	12:15	Hicham Mansouri and Theodore B. Trafalis (speaker) On-Line Reinforcement Learning Using Kernels
10	12:15	12:40	Leyuan Shi (speaker) Nested Partitions Optimization Framework and its Applications
11	12:40	13:05	Leo Liberti (speaker), Carlile Lavor, Nelson Maculan and Marco Antonio Chaer Nascimento Solving Hartree-Fock Equations with Global Optimization

Saturday, 16th June

1	8:00	8:25	Yannis Marinakis (speaker), Magdalene Marinaki, Michael Doumpos, Nikolaos Matsatsinis and Constantin Zopounidis A New Metaheuristic Algorithm for Cluster Analysis
2	8:25	8:50	Jose A. Egea (speaker), Emmanuel Vazquez, Julio R. Banga and Rafael Marti Improved Scatter Search for the Global Optimization of Computationally Expensive Dynamic Models
3	8:50	9:15	Panos M. Pardalos (speaker) Analysis of Greedy Approximation with Non-submodular Potential Functions
4	9:15	9:40	Julien Villemonteix (speaker), Emmanuel Vazquez, Maryan Sidorkiewicz and Eric Walter Gradient-Based IAGO Strategy for the Global Optimization of Expensive-to-Evaluate Functions and Application to Intake-Port Design
5	9:40	10:05	Kurt M. Anstreicher (speaker) SDP versus RLT for Nonconvex QCQP
6	10:05	10:30	Pham Dinh Tao (speaker), Nguyen Canh Nam and Le Thi Hoai An An Efficient Combined DCA and B&B using SDP Relaxation for Globally Solving Binary Quadratic Programs
	10:30	11:00	Coffee Break
7	11:00	11:25	Stefan Vigerske (speaker) LaGO - Branch and Cut for Nonconvex MINLPs
8	11:25	11:50	L.G. Casado (speaker), J.A. Martinez, I. Garcia and E.M.T Hendrix Development of a Parallel Advanced Multidimensional Interval Analysis Tool for Global Optimization (PAMIGO)
9	11:50	12:15	László Pál (speaker), Tibor Csendes, Oscar H. Sending and Julio R. Banga Improvements on the GLOBAL Optimization Algorithm with Numerical Tests
10	12:15	12:40	Dario Izzo and Tamás Vinkó (speaker) Learning the Best Combination of Solvers in a Distributed Global Optimization Environment

Conference Abstracts

A Semi-Deterministic Global Optimization Method for Credit Portfolio Optimization under Constraints

Benjamin Ivorra (speaker), Bijan Mohammadi and Ángel Manuel Ramos del Olmo

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Semi-deteministic optimization methods

We consider $J:\Omega\to\mathbb{R}$ with $\Omega\subset\mathbb{R}$. We make the following assump tions: $J\in C^1(\Omega,\mathbb{R})$ and is coercive. The infimum of J is denoted by J_m (when J_m is unknown, we set J_m to a low value).

Many deterministic minimization algorithms can be seen as discrete dynamical systems coming from the discretization of first or second order Cauchy problems. On the other hand, global optimization can be considered as an over-determined Boundary Value Problem (BVP) for these problems. For instance, the steepest descent method leads to the following BVP:

$$T_v > 0 \text{ given}, \quad \dot{x}(t) = -\nabla J(x(t)), \quad x(0) = v, \quad J(x(T_v)) = J_m$$

The over-determination can be removed by considering the initial conditions υ as new variables to be found by the minimization of $h(\upsilon) = J(x_\upsilon(T_\upsilon)) - J_m$, where x_υ is the solution of the dynamical system starting from υ. This is solved with an original Semi-Deterministic Algorithm (SDA) which minimizes $h(\upsilon)$ using a multi-dimensional shooting method.

Application to credit portfolio optimization

Various version of this SDA have been validated on several industrial problems involving local minima such as: credit portfolio management, optical fiber synthesis, shape optimization of fast-microfluidic-mixer devices, temperature and pollution control in a bunsen flame, shape optimization of coastal structures …

During this presentation, we will focus on the application of our method to the improvement under constraints of various portfolio performances, in particular non-convex risk measures and profitability.

Global Optimization of Higher Order Moments in Portfolio Selection

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We discuss the global optimization of the higher order moments of a portfolio of financial assets. The proposed model is an extension of the celebrated mean variance model of Markowitz. Since asset returns typically exhibit excess kurtosis and are often skewed, and investors would prefer positive skewness and try to reduce kurtosis of their portfolio returns, the mean variance model (assuming either normally distributed returns or quadratic utility functions) might be too simplifying. The inclusion of higher order moments has therefore been proposed as a possible augmentation of the classical model in order to make it more widely applicable. The resulting problem is non-convex, large scale, and highly relevant in financial optimization. We discuss the solution of the model using two stochastic algorithms. The first is a simulated annealing (SA) approach where a solution is iteratively updated. SA has two main ingredients: first, white noise is added to the current solution in order to generate a new solution within the neighborhood within the current one. Second, a probabilistic acceptance criterion encourages improvements, but also allows impairments in order to escape local optima. The second is based on the asymptotic behaviour of a suitably defined Stochastic Differential Equation (SDE). The SDE consists of three terms. The first term tries to reduce the value of the objective function, the second enforces feasibility of the iterates, while the third adds white noise in order to enable the trajectory to climb hills. We use the two algorithms both to gain insight into the financial model as well as to understand the numerical performance of the two algorithms.

Global Optimization in Computer-Assisted Proofs

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In several cases theoretical mathematical proofs pose a yes or no question whether a set containment relation of the form $T(A) \subseteq B$ holds [1, 2, 4] Here a set A described e.g.\ by nonlinear equations is transformed by a nonlinear map T (in our cases it is given by a dynamic system, a differential equation). The checking itself is made by an interval arithmetic based verified adaptive subdivision method. This verification technique proved to be fast enough on the investigated problem instances. Now optimization comes into the picture when the problem setting is not precise in the sense that not all the coordinates and parameters of the investigated sets and the transformation are known. We defined a global optimization problem related to the above one in such a way that all zero solutions of it mean a positive answer for the asked question -- and the unknown problem parameters are also identified [5] For the solution of this global optimization problem we used a stochastic clustering multistart approach, GLOBAL [3]. Notice that this time it is not necessary to apply a verified solver. We used successfully the described technique -- for example -- to locate a region where the 2-nd and 3-rd iteration of a H\'enon map $H(x, y) = (1 + y - ax^2, bx)$ instance has a chaotic behavior, and to improve the published lower bound (0.338) of the topological entropy to 0.382 [2]. In the talk we provide details on the results achieved.

References

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Reliable Trajectory Design Through Evidence Theory and Multiobjective Optimisation

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In the early phase of a space mission design, it is generally desirable to investigate as many feasible alternative solutions as possible. At this particular stage, an insufficient consideration for uncertainty would lead to a wrong decision on the feasibility of the mission. Traditionally a system margin approach is used in order to take into account the inherent uncertainties within the subsystem budgets. The reliability of the mission is then independently computed in parallel. An iteration process between the solution design and the reliability assessment should finally converge to an acceptable solution.

By combining modern statistical methods to model uncertainties and global search techniques for multidisciplinary design, the present work proposes a way to introduce uncertainties in the mission design problem formulation. By minimising the effect of these uncertainties on both constraints and objective functions, while optimising the mission goals, the aim is to increase the reliability of the produced results.

Uncertainties are usually classified in two distinct categories, aleatory and epistemic uncertainty [1]. Aleatory uncertainty results from the fact that a system can behave in random ways while epistemic uncertainty results from the lack of knowledge about a system and is a property of the analysts performing the analysis. In the particular case of preliminary space mission design, analysts face both type of uncertainty. For example, the initial velocity of the spacecraft, the gravity model or the solar radiation present aleatory uncertainties. However, most of the parameters of the spacecraft subsystems are first assessed by a group of experts, expressing their opinion on ranges of values. The classical way to treat uncertainty is through probability theory. It is well suitable to mathematically model aleatory uncertainties, as far as enough data, experimental for instance, are available. Even though, the analyst still has to assume the distribution function and estimate its parameters. Moreover, the available data may be insufficient to construct an acceptable probability distribution. In this case, the uncertainty is in fact epistemic and not aleatory.

Probability fails to represent epistemic uncertainties because there is no reason to prefer one distribution function over another. When uncertainties are express by means of intervals, based on experts' opinion or rare experimental data, as it is the case in space mission design, this representation becomes even more questionable.

Here we propose to use Evidence Theory instead of probability theory to address this issue. Evidence Theory, developed by G. Shafer from A.P. Dempster's original work, has be proven to model adequately both types of uncertainty [2,3].

A general trajectory optimisation model is reformulated as a multiobjective optimisation problem in which both the original objective, for example the mass of the spacecraft, and the belief that the value of the objective function is true are maximised. The multiobjective optimisation problem is then solved with a population based optimiser that construct the Pareto front for the two objective. Some examples of robust design of low-thrust trajectories will illustrate the proposed approach.

References

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Global Optimization of Robust Chance Constrained Problems

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We propose a stochastic algorithm for the global optimization of chance constrained problems. We assume that the probability measure with which the constraints are evaluated is known only through its moments. The algorithm proceeds in two phases. In the first phase the probability distribution is (coarsely) discretized and solved to global optimality, using a stochastic algorithm. We only assume that the stochastic algorithm exhibits a weak* convergence to a probability measure assigning all its mass to the discretized problem. A diffusion process is derived that has this convergence property. In the second phase, the discretization is improved by solving a linear semidefinite programming problem. It is shown that the algorithm converges to the solution of the original problem. We discuss the numerical performance of the algorithm and its application to process design.

A New Method of Addressing Process Synthesis Containing Black-Box Functions

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Keywords: Global Optimization, MINLP, Noisy Variables, Black-Box, Kriging

Process synthesis problems lacking closed-form model equations are very difficult to solve when noisy input-output data are the only information available using black-box (BB) units. Derivative-based optimization methods can prematurely terminate at artificial optima due to gradient inaccuracy that motivates the use of surrogate models which are robust against the noise. The use of local models may lead to the discovery of suboptimal solutions, but global model building and sampling costs can become prohibitively high if many BB process units exist. The problem we are addressing in this work has the following form:

$$\begin{aligned} &\min F(x,y,z_1,z_2) \\ &\text{s.t.} \quad g(x,y,z_1,z_2) \le 0 \\ &\qquad h(x,y,z_1) = 0 \\ &\qquad z_2 = \Gamma(x) + \varepsilon \\ &\qquad \varepsilon \sim N(\mu,\sigma^2) \end{aligned} \qquad (1)$$

In this formulation, *x* and *y* represent continuous and binary variables, respectively. Deterministic output variables z_1 describe outputs whose modeling equations $h(x,y,z_1)$ are known. Stochastic output variables z_2 exist when the input-output functionality $\Gamma(x)$ is BB simulated by a deterministic output perturbed with noise. Synthesis equations are given by $g(x,y,z_1,z_2)$ which include design constraints, operating specifications, and logical relations. We propose a new methodology to efficiently solve process synthesis problems modeled as MINLP problems containing noisy variables and BB functions described in this manner.

Focusing on the optimization methods when these complications are present, sampling-based global zero-order methods such as DIRECT (Jones et. a1 1993), MCS (Huyer & Neumaier, 1999), and DE (Storn & Price, 1995) can be used, but convergence may be asymptotic. In order to accelerate convergence and obtain an understanding of system behavior, gradient-based techniques can be sequentially applied to inexpensive fitted local models known as response surfaces (Myers & Montgomery, 2002). Recently, we developed an algorithm based on local response surfaces employing 1) adaptive experimental designs to retain feasibility, and 2) projection of the n-dimensional response surface onto constraints, thereby addressing the solution of nonlinear programs (NLP) in higher dimensions with arbitrary convex constraints (Davis & Ierapetritou, 2006). In contrast to response surfaces which are local models, a kriging predictor is a global model employing normally distributed basis functions, so both an expected sampling value and its variance are obtained for each test point (Goovaaerts, 1997). After prediction and variance mappings are obtained, the kriging predictor is updated using sampling in high-variance regions. Once convergence is achieved in the average value of the predictor, the algorithm which is using response surface is applied to promising local regions in order to identify the global optimum. If the problem dimensionality increases due to the presence of multiple BB units, kriging model building costs significantly increase, an issue addressed in our proposed methodology.

The central idea of the proposed algorithm for the solution of problem (1) is to use a Branch-and-Bound framework whereby for each relaxed NLP, kriging predictors built for each BB process unit are used to

identify promising regions for local search, which then serve as starting neighborhoods for further optimization using sequential response surfaces. In order to reduce sampling and model building costs, coarse predictors are built during the early stages of optimization which are iteratively updated using RSM sampling data. Our proposed algorithm relies on the idea that tight LB/UB need not be determined during the early stages of optimization. As the kriging predictors are updated at subsequent nodes, the LB/UB accuracy increases, thereby ensuring that the integrality gap will be more reliable due to tighter LB/UB.

In order to refine the set of potential local optima and to find the global optimum, response surfaces are built around starting iterates centered within each promising region. Collocation points are generated for each continuous input X_{Ind} which is independent of noisy outputs from upstream process units, as well as for the relaxed binary variables. For a BB process unit P_j, its input collocation points x_j are determined from the outputs z_i of the upstream unit P_i. After minimizing the response surface for the objective in terms of x_{Ind} and the binary variables, another set of collocation points is generated around the new iterate. This process continues until convergence has been achieved in the objective, which serves as a lower or upper bound depending upon feasibility in the binary variables.

The kriging predictors are sequentially constructed in order of possible appearance in the synthesis flowsheet to determine which units have noisy outputs serving as inputs to another one downstream. First, a kriging predictor is generated for each noisy output of the first upstream BB process unit. Minimum and maximum values for the kriging predictors are then obtained in order to determine the expected operating ranges of this set of inputs to the next potential downstream unit. The feasible operating range for x_j, is given as $(z_{j,min}-3\sigma_{i,max}) \leq (z_i = x_j) \leq (z_{i,max} + 3\sigma_{i,max})$, where $\sigma^2_{i,max}$ represents the maximum variance of the kriging predictor for P_i. If P_j is also BB, another kriging predictor is generated based on a possibly smaller expected feasible region resulting from the extended operating range of z_i. The advantage of sequentially generating kriging predictors based upon information from upstream process units, as opposed to creating them independently from one another based on the predefined operating ranges, is that the sampling expense will be smaller for those BB units P_j which have extended operating ranges smaller than the predefined limits.

In this work we are using several numerical examples and synthesis problems in order to illustrate the proposed methodology.

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Global Optimization Models and Algorithms for the Management of Cascading Risks via Event Trees

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In this paper, we present a novel quantitative analysis for the strategic planning decision problem of allocating certain available prevention and mitigation resources to respectively reduce the failure probabilities of system safety features and the total expected loss arising in the aftermath of a hazardous event. Using an event tree optimization approach, the resulting cascading risk scenario problem is modeled as a nonconvex factorable program. We derive a tight linear programming relaxation along with several theoretical insights that serve to lay the foundation for designing a specialized branch-and-bound algorithm that is proven to converge to a global optimum. Computational experience is reported for a hypothetical case study and several other test problems to demonstrate the efficacy of the proposed algorithm.

An Incremental Approach to the Solution of Global Trajectory Optimisation Problems

Massimiliano Vasile, Matteo Ceriotti and Paolo De Pascale

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In recent times there has been a flourishing interest in methods and tools for preliminary mission analysis and design. In particular, the generation of a large number of mission alternatives that can serve as first guesses for more detailed and sophisticated analyses.

This interest is directly related to the modem approach to space mission design, which steps though phases of increasing complexity, the first of which is always a mission feasibility study. In order to be successful, the feasibility study phase has to analyse, in a reasonable short time, a large number of different mission options. Each mission option requires the design of one or more optimal trajectories. In mathematical terms, the problem can be seen as a global optimisation or as a global search for multiple local minima.

A typical example is the optimisation of multiple gravity assist trajectories. In this case a spacecraft exploits the encounter with one or more planets in order to increase or decrease its kinetic energy with respect to the Sun. For an accurate trajectory model, the number of alternative paths can grow exponentially with the number of encounters. Moreover finding an optimal planet-to-planet transfer is in itself a global optimisation problem due to the high number of local minima [1].

Solving the problem could be a challenge for every global optimisation tool. However, this class of global trajectory optimisation problems can be decomposed in subproblems of smaller complexity and solved incrementally adding one planet at the time. At each incremental step a portion of the search space can be pruned out.

Previous attempt to use an incremental pruning have employed a simplified trajectory representation and a grid sampling of each subproblem. This approach fails if the accuracy and complexity of the trajectory model are increased for two reasons: if a course grid and an aggressive pruning are used many optimal solutions are lost, on the other hand if a fine grid is used the computational time becomes unacceptable even for a limited number of planets.

In this paper we propose a different incremental approach in which grid sampling is substituted with a global search through a stochastic approach [2]. Each global search aims at finding not only the global optimum but also a number of local optima. Then, the neighbourhood of each local optima is preserved and the rest of the search space is pruned out.

We will show how the proposed stochastic search performs, for each subproblem, an effective exploration of the search space that allows an efficient and reliable global optimisation of the whole trajectory.

This approach will be compared to the direct application of known global optimisation tools to the whole trajectory and to the solution through grid sampling.

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Packing Circles and Convex Polygons into Area-Minimizing Rectangles

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A set of circles, convex pieces of circles, and rectangles are to be nested into a set of rectangular design plates to be produced or into a set of given plates of known geometric dimensions available on stock. The objective is to minimize trimloss. The design plates are subject to lower and upper bounds of their widths and lengths. The objects are free of any orientation restrictions. If a circle exceeds the dimensions of the plates it can be cut into two or three pieces.

If all nested objects fit into one design or given plate the problem can be described as a nonconvex nonlinear programming problem. We present a model formulation and a solution approach which solves this problem for a modest number of objects, for instance, 6 circles and 3 rectangles, in short time to global optimality.

If the number of objects cannot be nested in one plate, additional integer variables are needed to represent the allocation problem leading to a nonconvex mixed integer optimization problem.

We have successfully applied several solution techniques to solve this problem among them the Branch&Reduce Optimization Navigator (BARON) called from GAMS, a taylor-made Branch&Bound method for solving the allocation problem, and a column enumeration approach in which the columns represent feasible assignments.

We support the solution process by computing lower and upper bounds to the solution by constructing relaxed and tightened models.

Keywords: Global Optimization, mixed integer programming, column enumeration, Branch&Bound, cutting stock, nesting, overlap constraints, design problem

Column Enumeration based Decomposition Techniques for a Class of Non-Convex MINLP Problems

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Problems assigning projects to departments, activities to units, delivery orders to vehicles, or packing geometric objects to given areas are well known real world problems. Treating this type of problems mathematically can easily lead to non-convex mixed integer non-linear programming (MINLP) problems. Solving them is in general very challenging as they belong to the 'harder' cases of the NP-hard problems.

The non-convex MINLP problems we want to solve are assignment problems in which a set of n objects, $i \in I$, should be allocated to a set of resources $r \in R$. Each object i needs to be allocated to exactly one resource. Resource r can cover several objects. The allocation decisions are represented by binary variables indicating that an object i is allocated to a resource r. Examples are the vehicle routing problem in which orders are allocated to vehicles, or geometrical objects assigned to and cut from given steel plates.

The optimization problem to solve is given by min $\sum_r f(x,y,\alpha)$ with continuous variables $x \in \mathbb{R}^{n_c}$, integer vaiables $y \in \mathbb{R}^{n_d}$ and binary variables $\alpha \in \{0,1\}^{n_b}$. The constraints are given by

$$\begin{array}{l} g(x,y,\alpha) = 0 \\ h(x,y,\alpha) \geq 0 \end{array} \quad and \quad \sum_r \alpha_{ir} = 1 \quad ; \quad \forall i$$

In most cases this problem is non-convex. If there are many resources r to consider the problem becomes quickly very large and difficult to solve to global optimality.

If the assignment decisions are decoupled from the remaining constraints of the optimization problem, we propose to use a column enumeration approach. A column c is any index set $I_c \subseteq I$. As the number of columns grows exponentially in n, we can use a complete enumeration only for small values of n, e.g., smaller than 10 or 15. We obtain a decomposed problem with respect to the columns *c*. The master problem is a partitioning problem whose objective function coefficients are computed in a subproblem. The subproblem can be a LP, MILP, NLP or MINLP problem. The important property of the subproblem is that we can compute its exact global minimum in short time.

We will illustrate decomposition approach solving a packing problem with a non-convex NLP subproblem. Furthermore, some generalizations of this assignment problem are discussed, including to allow more general constraints.

Some Transformation Techniques with Applications in Global Optimization

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Signomial terms appear frequently in engineering optimization, making such problems difficult to solve to global optimality. In this paper some simple transformation techniques, applicable to such terms, are discussed.

The transformations, discussed in the paper, are especially useful when solving optimization problems including constraints which are composed of a convex and a signomial function. Such constraints can be transformed to convex form by the transformations. In addition, by approximating the inverse transformations by piecewise linear functions, it can be shown that these non-convex constraints can not only be convexified but also be underestimated. The latter property is important when developing global optimization approaches, since it allows us not only to convexifl and to underestimate the constraints, but also to transform certain non-convex problems, including signomial functions, to convex form, with a feasible region overestimating the feasible region of the original problem.

When the transformations are applied, the original non-convex feasible region is, implicitly, divided into convex sub-regions, by this approach, where each sub-region is defined by the binary variables used in the piecewise linear approximations of the inverse transformations.

With the given techniques, some general classes of non-convex MINLP (mixed integer non-linear programming) problems can be solved to global optimality. The global optimal solution of the original non-convex problem can be found by solving a sequence of convexified MINLP sub-problems. After each such iteration a part of the infeasible region is cut off, by updating the piecewise linear approximations of the inverse transformations. The algorithm terminates when a solution point is sufficiently close to or within the feasible region of the original problem. The principles behind the algorithm are given and a numerical example is given to illustrate how the global optimal solution is obtained with this approach.

Keywords: Transformation techniques; mixed integer nonlinear programming; signomial hnctions; global optimization**.**

A Multi-Scale Approach to Global Optimization for Molecular Conformation Problems

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Molecular conformation problems such as protein folding and crystal structure determination are considered to be among the most challenging problems for global optimization algorithms. This is because they exhibit many local minima and saddle points and because the number of stationary points generally grows exponentially as the number of degrees of freedom increases. However, this particular class of global optimization problems is often characterized by two distinct geometries - noisy or rugged objective function behavior at small length scales and an objective function that has funnel shaped or non-quadratic geometry at large length scales - suggesting that these problems are ideally suited for multi-scale global optimization methods.

In this talk a new and completely deterministic multi-scale methodology for global optimization is described. The overall multi-scale methodology is based on alternating between small-scale and large-scale optimization calculations to build both local and global representations of the objective function. A terrain method is used at the small length scale to find local sets of stationary and singular points that lie in valleys and to gather average gradient and Hessian matrix information. On the other hand, a funneling method is used at the large length scale to build funnel approximations of the large-scale geometry and to make large conformational moves on the objective function surface.

The key to the success of our multi-scale global optimization approach lies in the coordinated and intelligent use of information at both length scales. At the small scale average information is gathered by using the mean value theorem to average both gradient and curvature information along the terrain path. Experience shows that it is extremely important to gather information along the low-lying valleys on rough or noisy objective function surfaces - regardless of location. This averaged information is critical in initializing the funneling calculations that are used at the large length scale. Funneling calculations are initialized using averaged information from two arbitrary regions on the objective function surface. This defines the communication from small to large length scale. Subsequent funnel iterations use a mixture of averaged and point-wise gradient and Hessian matrix information. The funneling calculations, which have an asymptotic rate of convergence that is quadratic, are forced to produce a monotonically decreasing sequence of objective function values and are converged to a minimum because they are so much faster than the small-scale terrain calculations. This often results in large conformational changes during the funneling phase of the optimization. Moreover, when the funnel calculations converge to a local minimum, the multi-scale algorithm returns to the small-scale terrain calculations. This defines communication from the large to small length scales, where a new set of stationary and singular points, an associated terrain path, and averaged gradient and Hessian matrix information along that terrain path are computed. Our methodology then replaces the point-wise gradient of zero at the computed local minimum by non-zero valued average gradient information in the vicinity of the local minimum and it is in this way that the proposed multi-scale approach avoids getting trapped at local minima on the objective surface. This also forces the next set of funneling calculations, which are monotonically decreasing by design, further down the funnel. Termination occurs when the multi-scale methodology can go no longer reduce the value of the objective function during a funneling phase.

A number of interesting molecular conformation problems are used to illustrate the reliability and efficiency of our multi-scale global optimization methodology. These applications include benchmark

problems from the class of Lennard-Jones (LJ) clusters - specifically LJ_{I3}, LJ_{I9}, and LJ_{38} - as well as problems in determining the crystal structure of n-alkane waxes (i.e., whether the global minimum corresponds to a liquid-like rotator phase or a low temperature ordered solid phase). Numerical results show that the proposed multi-scale global optimization approach is extremely reliable and always finds the global minimum. It is also computationally efficient - often requiring only small numbers of stationary and singular points at the small length scale (typically 10-1 5) and converging in one or two sets of large-scale funneling calculations. Key features of our approach and interesting aspects of various applications are illustrated geometrically.

Global Optimization Approaches for the Synthesis of Regulatory Networks

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The transcription of genes is regulated by DNA-binding proteins (transcription factors, TF) that attach to the promoter region and regulate the expression of the corresponding genes. Targeting expression by controlling the regulatory process through the corresponding transcription factors is emerging as a viable option for the identification of drug targets in general [1,2]as well as the control of specific disease conditions [3]. In recent years significant efforts have been made experimentally, and computationally, to identify transcription factors, their target genes and the interaction mechanism that control (regulate) gene expression [4]. An important technique for elucidating binding interactions is chromatin immunoprecipitation (Chip) experiments [5]. However, physical binding of a TF is a necessary but not sufficient condition for transcription initiation and regulation. Due to various complex post-translational modifications as well as interactions among multiple TFs the measured expression level of regulatory genes does not reflect the actual activity of the TFs themselves. Therefore, regulator transcription levels are generally not appropriate measures of transcription factor activity (TFA). Recently, methods combining TF-gene connectivity data and gene expression measurements have emerged in order to quantify these regulatory interactions. Prominent examples are the decomposition-based methods which combine Chip and microarray data and inversion of regression techniques to estimate TFAs [6-9]. Singular Value Decomposition and regression methods were combined order to reverse engineer regulatory networks, whereas in [11] promoter elements were linearly combined to quantify the contribution of the promoter architecture on a gene's expression. Network Component Analysis (NCA) [12-16] as introduced as an alternative for quantifying the strength of the regulatory interactions and for elucidating true TFAs, [17] explore a similar linear superposition of expression profiles and TFA combined appropriately using binding affinities in lieu of stoichiometric coefficients and a Bayesian error analysis of an, effectively, linear method was presented in [17]. The main goal of this reverse engineering is to identify the activation program of transcription modules under particular conditions [18] so as to hypothesize how activation/deactivation of expression can be induced/suppressed [19]. A fundamental difference among the methods is whether the weights of the approximation should be estimated through regression [12-16] or associated with binding affinities [17]. Aside from the development of descriptive models hat correlate TFA and expression of target genes, a critical question becomes how to identify those TFs that significantly contribute to regulation and should be modulated. Along those lines [8] speculate that the mRNA profile of the target gene should be similar to the reconstructed TFA for the regulating proteins, whereas [17] claim that accurate binding information should lead to robust TFA reconstructions.

A major problem associated with the reverse engineering of genetic networks from microarray and binding data, is how to reliably find critical and informative regulatory interactions in a systematic way. In order to address this problem we propose the development of a mixed-integer non-linear problem aiming at the synthesis of genetic regulatory networks with the following main characteristics:

1. A superstructure of the network topology is determined computationally exploring the concept of position weight matrices [20], with the primary difference being that the output of our algorithm will not be a binary 1-0 matrix in which the transcription factor binds, or the transcription factor does not bind, but rather a probability matrix in which under a certain threshold, the probability of the transcription factor binding is zero, but over the threshold, the

transcription factor binds with a certain non-zero probability. The transcription factor binding matrices were obtained from TRANSFAC [21].
2. The positive of negative character of the regulatory interactions between transcription factors and genes is explicitly modeled in our framework, using appropriate binary variables, thus allowing the identification and quantification of specific contributions.
3. The complexity of the regulatory network is explicitly controlled and multiple, alternative, structures are systematically determined.

We formulate the problem of designing regulatory structures as a non-convex MINLP with the main source of non-convexities be a bilinear product between the binary variables indicating the positive/negative regulation and the activity of the corresponding transcription factor. The solution methodology follows two distinct paths. First, we explore effective linearization of the formulation using the reformulation proposed by [22] where these non-convexities can be eliminated by introducing a new set of continuous variables. We further evaluate the effectiveness of the Global Optimum Search (GOS) methodology proposed by Floudas and coworkers [23] which involves a decomposition of the variable set into two sets: complicating and non-complicating variables. This results in a decomposition of the constraint set leading to two sub-problems. The decomposition of the original problem induces special structure in the resulting sub-problems and a series of these sub-problems are then solved, using the Generalized Benders' Decomposition technique, to determine the optimal solution.

The effectiveness of the solution methodology for the regulatory network reconstruction is demonstrated through a series of test case examples involving synthetic data [24], yeast cell cycle data [17] and finally a burn-induced inflammatory rat animal study [25]. Our results indicate the advantages of the modeling methodology and the effective solution in terms of discovering significant and informative components of the regulatory structure. We discuss the comparison among the two approaches and demonstrate the advantages of the GOS algorithm. We finally demonstrate the potential advantages offered by the systematic reconstruction of alternative regulatory structures in terms of identifying robust reconstruction of transcription factor activities that could be used a putative therapeutic interventions targets.

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A New Approach to Fluence Map Optimization in IMRT

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The goal of intensity-modulated radiation therapy (IMRT) for cancer treatment is to maximize the radiation absorbed by tumors and minimize that absorbed by surrounding organs. The current clinic practice uses so-called dose-volume constraints to achieve balances between conflicting goals, but at the same time creates difficult, large-scale, global optimization problems of combinatorial nature. We propose a novel formulation for this problem and a greedy algorithm for its solution. We will report our numerical results on clinic cases, comparing our approach to the one employed by most commercial systems. We find that our approach produces treatment plans of competitive quality with a significant improvement in computational performance.

A Note on Funnel Functions

K.M. Rajesh (speaker) and Asim K. Pal

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Funnel functions are of growing interests in the optimization community, especially in fields such as computational chemistry and biology. The objective functions of many problems including protein folding, protein-protein docking, virus capsids, molecular clusters (such as Lennard-Jones and Morse clusters) and densely packing geometrical objects are believed to be 'funnel-like' (Addis, 2004; Addis, Locatelli and Schoen, 2005; Wales, 2003,2005). Funnel functions were first suggested while studying the protein folding problem (Leopold, Montal and Onuchic, 1992; Bryngelson, Onuchic, Socci and Wolynes, 1995). These are nonconvex continuous functions in the unconstrained domain characterized by a particular arrangement of local minima.

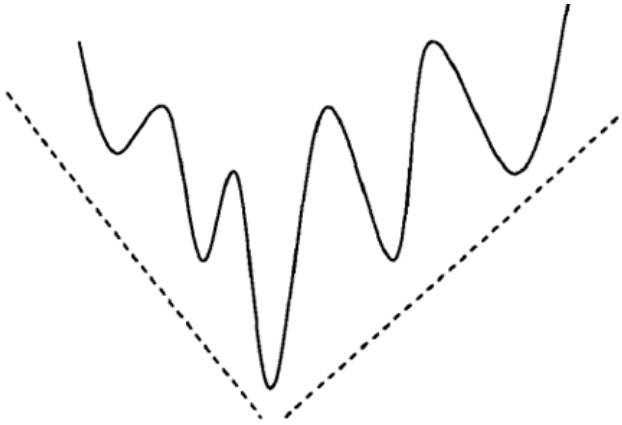

Figure 1a: A single funnel in one dimension

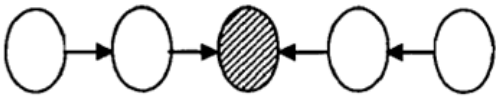

Figure 1b: Directed graph representation of the function given in Figure 1a

Consider the one dimensional function given by the continuous line in Figure la. In this function, for every local minimum which is not the global minimum, there is a neighborhood basin containing a minimum with a lower function value. This type of arrangement of the local minima approximates to the shape of a funnel, given by the broken line in Figure la. Hence, such functions were called funnel-like. Figure lb represents the same function using a directed graph. Funnel bottom is represented by the shaded node here. Locatelli (2005) discusses the multilevel structure of global optimization functions. According to this, the function in Figure la would be a single funnel. Algorithms which work on the local minimum mapping of the objective function are considered efficient for funnel functions (Wales and Doye, 1997; Leary, 2000; Addis, 2004)

There is no widely accepted definition of funnel functions in the literature. However, there is one definition available in Grosso, Locatelli and Schoen (2005). This definition uses directed graphs.

According to this definition, a funnel bottom would be a node with no outgoing arcs. A funnel is a set of local minima characterized by the fact, that for each of them there exists at least one decreasing sequence of 'neighbour' local minima along a path leading to the funnel bottom.

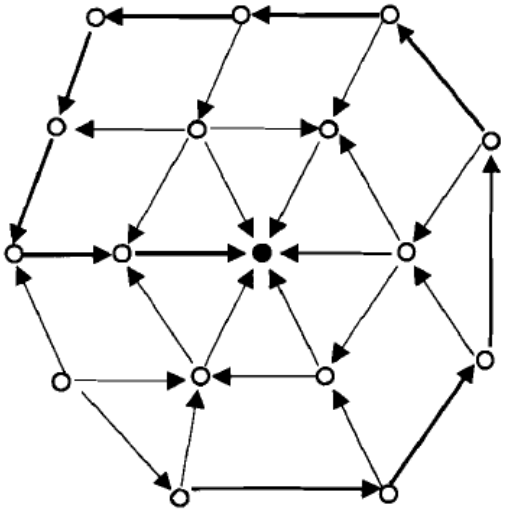

Figure 2a: Funnel

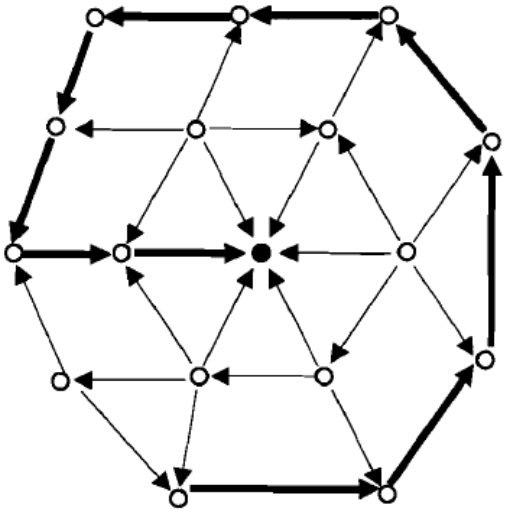

Figure 2a: Funnel according to the definition given in Grosso et al (2005)

In this paper we discuss some limitations of the definition of funnel given in Grosso et a1 (2005). We find that in one dimension this definition represents 'funnel-like' functions. But as we increase the dimensions, this definition would not result only in 'funnel-like' functions. The functions satisfying this definition may include various categories of functions, many of which are even difficult to visualize even in two dimensions. To illustrate this point, refer to directed graphs given in Figures 2a and 2b. Figure 2a represents a function which is 'funnel-like', where as, it is arguable to categorize Figure 2b as funnel-like, because the function does not approximate to a funnel. The function in Figure 2b would however satisfy the definition of funnel given in Grosso et a1 (2005). Note that any local minima in Figure 2b has a maximal descent sequence which terminates at the funnel bottom. To illustrate this point, one long maximal descent sequence has been highlighted in Figure 2b. We find that popular algorithms for funnel functions, such as Monotonic Basin Hopping (MBH) (Leary, 2000) and Local Optima Smoothing (LOS) (Addis, 2004), will become inefficient for these categories of funnel functions. We argue that the more recent simplex based search algorithms, Nelder Mead Local Search (NMLS) and NMLS-Shrink variant (NMLS-S) (Rajesh, 2006) try to overcome the problems encountered by MBH and LOS. However, it is to be mentioned that the categories of functions where NMLS and NMLS-S would perform worse than
MBH and LOS, are still not known to us.

Keywords: Funnel functions, Local minima mapping, Monotonic Basin Hopping, Local Optima Smoothing, Simplex based search, Nelder Mead Local Search, NMLS-Shrink variant

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Vaccination Strategies Dynamics of Population Groups with Distinct Perceived Probabilities of Infection

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In this paper we study the strategic interaction of groups in a=20 heterogeneous population for certain infectious diseases. The=20 heterogeneity of the population groups is dictated by their varying=20 perceived relative risks of infection versus vaccination, as well as by=20 their distinct perceived probablilities of being infected, given the=20 vacine coverage in the population as a whole is p. This is a direct generalization of the work presented in Cojocaru, Bauch=20 and Johnston (Bulletin of Mathematical Biology 2006). We will use game=20 theory, projected dynamical systems and variational inequality theories as=20 our mathematical methodologies for this study. Previous game theoretic=20 analyses of vaccination strategies in homogeneous populations have been=20 considered by Bauch (2005) and Bauch and Earn (2004) .

Finding Optimal Feeding Schedules in Pig Production

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For many decades, linear programming has been used to find minimum cost diets, notably in the chicken and pig meat industries. More recently, animal growth models together with nonlinear optimization methods have been used to find feeding schedules which simultaneously minimise feed costs and maximise market return, so maximizing gross margin. Genetic algorithms can handle these problems, albeit slowly. In this paper we study the particular nature of the objective function (for pig meat production) and develop a global optimisation algorithm tailored to its discontinuous structure. We also demonstrate the use of stochastic programming to cope with a changing price schedule.

The Interacting-Particle Algorithm with Dynamic Heating and Cooling

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A common issue for stochastic global optimization algorithms is how to set the parameters of the sampling distribution (e.g. temperature, mutation/cross-over rates, selection rate, etc) so that the samplings converge to the optimum effectively and efficiently. We consider an interacting-particle algorithm and develop a meta-control methodology that analytically guides the temperature parameter of the algorithm to achieve desired performance characteristics (e.g. quality of the final outcome, algorithm running time, etc). The interacting-particle algorithm is population-based like genetic algorithms and also has analogies to simulated annealing. The algorithm moves N particles inside the feasible set based on an N-particle exploration mechanism and an N particle selection mechanism. We implement the exploration phase using the Hit-and-Run sampler. The temperature parameter controls the N-particle selection mechanism. As this parameter approaches zero the particles become more concentrated around the global optima.

The meta-control methodology tunes algorithmic parameters during the course of the algorithm by incorporating the parameter effects into the algorithm dynamics. The main aspect of the meta-control methodology is to formulate an optimal control problem where the fractional change in the temperature parameter is the control variable. The criterion of the optimal control problem includes the expected objective function value of the particles, the spread of the particles, and the algorithm running time. The state of the control problem reflects the probability density of the particles and the state dynamics depends on N-particle mechanisms. In each iteration of the interacting-particle algorithm, we obtain information about the locations of the particles and the corresponding objective function values. From these observations we estimate the state of the control problem. We then solve a control problem that determines the change in the temperature parameter for the next iteration of the interacting-particle algorithm. We implement N-particle exploration and N-particle selection mechanisms with the new temperature, obtain new observations from particles and resolve the optimal control problem to determine the next iteration's temperature.

Our numerical results indicate that with this control methodology the temperature fluctuates (both heating and cooling) during the progress of the algorithm to meet our performance measures.

Tight Convex Underestimators for C^2-Continuous Problems

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Keywords: Convex Underestimation; αBB Theory; Global Optimization

Convex underestimation of nonconvex functions is of fundamental importance for Deterministic Global Optimization algorithms that utilize a Branch and Bound scheme. The tightness of the underestimators to the original function is directly linked with the computational efficiency of the optimization methods. For the case of general nonconvex functions, that do not exhibit some special structure that could possibly be exploited, one can use the convex underestimators based on the αBB theory [1, 2, 3]. In order for these underestimators to be constructed, one needs to have information on the bounds of the elements of the function's Hessian matrix, which could be obtained by performing interval arithmetic calculations. The method would benefit from shrinkage of the domain under consideration and this was firstly exploited in the $\rho - \alpha$BB method [4], where a piecewise approach was utilized. The method proposed partitioning of the domain into many subdomains and construction of the corresponding αBB underestimator for each one. These underestimators, although not valid for the entire domain, are much tighter to the original function in their respective subdomains. A hyperplane is subsequently added to each one of these underestimators and is selected in such a way, so that the overall underestimator produced is continuous and smooth (c'-continuity).

In our proposed approach we construct these αBB underestimators, but instead of adding hyperplanes we identify those tangential line segments that, in combination with convex parts of the original underestimators, constitute a c'-continuous convex underestimator that is valid for the overall domain under consideration. One can also consider only the lines defined by the linear segments, thus coming up with a piecewise linear underestimator, which can easily be incorporated in the NLP relaxation as a set of linear constraints.

This methodology, which is directly applicable to univariate problems, can be extended to multidimensional problems through proper projections of the multivariate αBB underestimators into one-dimensional spaces. Furthermore, since our method utilizes projections into lower-dimensional spaces, we explore ways to recover some of the information lost in this process. In particular, we apply our method after having transformed the problem in an orthonormal fashion. This leads to the construction of even tighter underestimators, through the accumulation of additional valid linear cuts in the relaxation. Improvements are observed both in the quality of lower bound obtained, as well as in the tightness of the underestimator across the whole domain under consideration [5].

The method has been tested on large collections of univariate and multivariate test problems. In most cases, the lower bounds obtained are close to the global minimum thus eliminating the need for any branching at all.

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An Analytical Method for derivation of the Steiner Ratio of 3D Euclidean Steiner Trees

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We stress the convenience of some analytical methods [1, 2] for calculating the Steiner Ratio of finite sets of points in $\mathbb{R}^3$. We also emphasize the usefulness of these methods for comparison of the results obtained for points evenly spaced along a right circular helix with a well-known algorithm [3]. This algorithm is adequate for calculating the Euclidean Steiner Trees in any dimension. The NP-hard characteristic of this problem shows itself in the time necessary for constructing these trees. Some useful experiments with this algorithm have been done with finite sets of points in $\mathbb{R}^3$. We now take into consideration the possibility of connecting all the points by a smooth and continuously differentiable curve such that all the points stand as evenly spaced along it. We then assume the existence of this curve and we consider a sequence P_j, $0 \leq j \leq$ n -1 of n consecutive points. We define the subsequences

$$(P_j)_{m,l_{Pmax}} : P_j, P_{j+m}, P_{j+2m}, \ldots, P_{j+l_{Pmax}m}. \tag{1}$$

The generic element is P_{j+lpm}, $0 \leq lp \leq \mathrm{lp}_{max} = \left[\frac{n-j-1}{m}\right]$ and the square brackets $[x]$ stand for the greatest integer value $\leq x$. In this representation, $(P_0)_{1,n-1}$ is the original sequence of consecutive points. We now consider, instead of this last sequence, a new sequence of n points which is the union of the subsequences above

$$\mathbb{P}_m = \bigcup_{j=0}^{m-1} (P_j)_{m,l_{Pmax}}. \tag{2}$$

The construction above is independent of coordinate representation but we assume an Ansatz for the coordinates of the points in order to favour the subsequent derivation of an analytical expression of the Steiner Ratio (1), or

$$P_{j+l_P m}(\omega) = (\cos(j + l_P m)\omega, \sin(j + l_P m)\omega, (j + l_P m)F(\omega)). \tag{3}$$

If the curve is a right circular helix, we have,

$$F(\omega) = \alpha\omega \tag{4}$$

where $2\pi\alpha = \rho$ is the pitch of the helix.
In this case, some exhaustive computational experiments lead to an analogous representation for the subsequences of Steiner Points,

$$S_{k+l_S m} = (r_m(\omega)\cos(k + l_S m)\omega, r_m(\omega)\sin(k + l_S m)\omega, \alpha(k + l_S m)\omega). \tag{5}$$

The functions $r_m(\omega)$ are obtained from the condition of the edges meeting at 120° on each Steiner point [4]. We get,

$$r_m(\omega) = \min\left\{1, \frac{m\alpha\omega}{\sqrt{A_m(A_m+1)}}\right\}, \quad A_m = 1 - 2\cos(m\omega) \ . \tag{6}$$

The Steiner Ratio Function is written as

$$\rho(\omega,\alpha) = \mathrm{Max}_{(m)}\left(\frac{1+\alpha\omega\sqrt{\frac{A_1}{A_1+1}}}{\sqrt{m^2\alpha^2\omega^2 + A_m + 1}}\right), \quad A_1 = 1 - 2\cos(\omega) \ . \tag{7}$$

This method can be applied to the generic Ansatz for discrete set of points belonging to conoidal curves of eq.(3). The problem of derivation of an analytical formula for Euclidean Steiner Trees in $\mathbb{R}^3$ would be solved if the constancy of the tree topology in the transition from a cylindrical to an amorphous configuration could be proved.

Keywords: Steiner Ratio, Analytical Method, Euclidean Steiner Trees.

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Fast and Tight Polynomial Bounds Based on Bernstein Expansion

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A new method for the representation and computation of Bernstein coefficients of multivariate polynomials is presented. It is known that the coefficients of the Bernstein expansion of a given polynomial over a specified box of interest tightly bound the range of the polynomial over the box. The traditional approach, however, requires that all Bernstein coefficients are computed, and their number is often very large for polynomials with moderately-many variables. A new method represents the coefficients implicitly and uses lazy evaluation so as to render the approach practical for many types of large polynomials typically encountered in global optimization problems; the complexity becomes nearly linear with respect to the number of terms in the polynomial, instead of exponential with respect to the number of variables.

These range-enclosing coefficients can be employed in a branch-and-bound framework for solving constrained global optimization problems, either as constant bounds used for box selection, or to construct affine underestimating bound functions. If such functions are used to construct relaxations for a global optimization problem, then sub-problems over boxes can be reduced to linear programming problems, which are easier to solve. Some examples will be presented and the software used will be introduced.

On the Min-Max Graph in Finite and Semi-Infinite Optimization

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We consider finite dimensional smooth optimization problems with compact connected feasible set. A variable (= Riemannian) metric defines an ascent and descent semi-flow. This gives rise to a bipartite digraph on the set of local minimizers and maximizers. (min-max graph). Active set strategy may cause a stable obstruction to the connectedness of the min-max graph. However, by means of an automatic constraint-adaptation of the metric the min-max graph becomes generically connected. In case of a single smooth inequality constraint we give an explicit formula of the metric adaptation. In case of finitely many constraints we propose a logarithmic pre-smoothing and for semi-infinite optimization we discuss a mollifier-pre-smoothing.

This is joint work with Oliver Stein.

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Existence and construction of polyhedral convex envelopes.

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Convex envelopes are a very useful tool in global optimization. However finding the exact convex envelope of a function is a difficult task in general. This task becomes considerably simpler in the cases where the domain is a polytope and the convex envelope is vertex polyhedral, i.e., has a polyhedral epigraph whose vertices correspond to the vertices of the domain.

We describe very general conditions and characteriztions for the existence of a vertex polyhedral convex envelope of a function on a polytope P. The complexity of the construction of such polyhedral envelopes is exponential in the dimension of the polytope in general. However, we show how to construct efficiently such envelopes in low dimension. Furthermore, we show some cases where the convex envelope can be constructed in time polynomial in the dimension of P.

Our theory extends and unifies several results previously obtained for special cases of this problem.

An Interior Point Newton Method for General Bounded Linear Complementarity Problems

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In this paper an algorithm will be presented to solve bounded linear complementarity problem (LCP) characterized by general coefficient matrices. The algorithm finds a complementarity point for a nonmonotone LCP by a primal Interior Point Newton method with a barrier function. The algorithm defines a convexification of a suitable barrier function, through a normalization and transformation procedure.

The outline of the paper is the following. After the introduction, in section two the algorithm will be described, while in the following section convergence results will be given and it will be shown that a solution can be found in polynomial time. In section four experimental results, showing in particular how this algorithm can determine global minima will be presented and appropriate conclusions will be drawn in section five.

Branch and Bound Algorithm for Multidimensional Scaling with City Block Metric

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Multidimensional scaling (MDS) is a technique for exploratory analysis of multidimensional data widely usable in different applications. Pairwise dissimilarities between n objects are given by the matrix (δ_{ij}), $i, j = 1, \ldots, n$. A set of points in an embedding space is considered as an image of the set of objects. Normally, an m-dimensional embedding metric space is used, and $\mathbf{x}_i \in R^m$, $i = 1, \ldots, n$ should be found whose inter-point distances fit the given dissimilarities. The problem of construction of images of the considered objects is reduced to minimization of an accuracy of fit criterion, e.g. of the most frequently used least squares *STRESS* function.

In the present paper MDS algorithms based on *STRESS* criterion with city block distances in the embedding space are considered. *STRESS* normally has many local minima. In the case of city block distances it can be non differentiable even at the minimum point. Therefore MDS with city block distances is a difficult high dimensional $\left(\mathbf{x} \in R^N, N = n \times m\right)$ global optimization problem.

If city block distances are used, *STRESS* is piecewise quadratic and its structure is favorable to apply a two level minimization algorithm: a problem of combinatorial optimization at the upper level and a problem of quadratic programming at the lower level. The number of feasible solutions of the upper level combinatorial problem is approximately $(n!)^m/(2^m m!)$. Explicit enumeration of all solutions is not computationally tractable for all but smallest problems. Evolutionary search can be applied.

In the present paper a branch and bound algorithm for solution of the upper level combinatorial problem is proposed to solve middle size problems exactly. The lower bound of the objective function is found solving MDS problems of smaller size - when only part of n objects are considered.

A Combined DCA - GA for Constructing Highly Nonlinear Balanced Boolean Functions in Cryptography

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Keywords: Cryptography, Boolean function, nonlinear balanced Boolean function, nonlinearity, Genetic Algorthim, Hybrid Genetic, DC programming, DCA, mixed 0-1 polyhedral convex program, exact penalty.

Substitution boxes, aka S-Boxes, are a key component of modem crypto-systems. Several studies and developments were carried out on this problem in the last few years. The robustness of block ciphers rely on qualities of such boxes such as non linearity and imbalance. This work is concerned with the construction of highly nonlinear balanced Boolean functions, which is an interesting and open question in Cryptography. A deterministic optimization model which is the minimization of a polyhedral convex function on a convex polytope with 0-1 variables is introduced. A local deterministic optimization approach called DCA (Difference of Convex functions Algorithm) is investigated. For finding a good starting point of DCA we propose two versions of a combined DCA - GA (Genetic Algorithm) method. Preliminary numerical simulations prove that DCA is a promising approach for this problem. Moreover the combination of DCA-GA improves the efficiency of DCA and outperforms other standard approaches.

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On-Line Reinforcement Learning Using Kernels

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In most studies conducted involving reinforcement learning (RL), the states and actions sets are considered to be finite and the cardinality of each set is fixed. Moreover, the techniques used to solve this type of problems require a huge amount of resources to find an optimal policy. Therefore, most of the models available need an off-line calculation. However, in real world problems, the environment might vary and include new states or actions that were not accounted for before. Hence, a policy that was optimal for a previous environment might not be optimal anymore. In this paper, we propose a methodology that applies the support vector clustering to reduce the cardinality of the set of states. Issues of computing optimal parameters using global optimization are also discussed. Then, we solve the new RL using the reduced states. Once a new state comes, we perform a test, using clustering, to check if we need to recalculate the optimal policy or no. The policies obtained are near-optimal policies and the more clusters we have the better is the policy. We used a fictional city evacuation scenario to test the efficiency of our method.

Nested Partitions Optimization Framework and its Applications

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Designing and operation of complex large-scale systems such as transportation systems, manufacturing systems, supply chain networks, and health care systems are very difficult tasks. Many contributing factors exist; chief among them is the exponential explosion of alternatives normally leading to NP-hard optimization problems. In the case of stochastic optimization, the situation is further complicated by randomness. We have recently developed a new framework called Nested Partitions (NP) for global optimization. NP uses partitioning, random sampling, selection of a promising index, and backtracking techniques to create a Markov chain, which has been proven with probability one to converge to a global optimum. One important feature of the NP method is that it can combine global search and local search (domain knowledge or heuristic) procedures in a natural way. The NP method is also highly matched to massively parallel processing capabilities. The global and parallelism nature of the optimization framework provides an efficient and effective platform for information sharing and exchange during search procedure.

Solving Hartree-Fock Equations with Global Optimization

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The quantum behaviour of atoms and molecules, in the absence of relativistic effects and external perturbations, is determined by the time-independent Schrödinger equation:

$$H\Psi_n = E\Psi_n,$$

where H, the Hamiltonian operator of the system, represents the total energy (kinetic + potential) of all the particles of the system. Analytical solutions for this equation are only possible for very simple systems. Hence, for the majority of problems of interest, one has to rely on some approximate model. In the Hartree-Fock model, the electrons in atoms and molecules move independently of each other, the motion of each one of the electrons being determined by the attractive electrostatic potential of the nuclei and by a repulsive average field due to all the other electrons of the system. In this model, the approximate solutions Φ_n, of Eq.() are anti-symmetrized products of one-electron wave functions $\{\varphi_i\}$ (also called orbitals), which are solutions of the Hartree-Fock (HF) equations for the system under study. Each orbital φ_i can be expanded in a complete basis set $\{x_s\}_{s=1}^{\infty}$. In order to transform the HF equations into a less cumbersome algebraic problem, we only consider a finite subset $\{x_s \mid s \leq b\}$ of the basis, and we use it to approximate the orbitals. The need for optimization arises because we need to find a set of coefficients c_{si}, for s = 1, . . . , b and i = 1,. . . , n, such that for all $i \leq n$ the function

$$\bar{\varphi}_i = \sum_{s=1}^{b} c_{si}\chi_s$$

is a good approximation of the i-th spatial orbital φ_i. The method most usually applied to the Hartree-Fock equations iteratively solves a set of linear equations to find the coefficients c_{si}. This method, however, has three main limitations: there is no guarantee that the set of coefficients c_{si} found by the method are a globally optimal such set; it depends on an initial solution being available (starting guess); the occupation number of all orbitals must be provided. We overcome these limitations by formulating this as a nonconvex optimization problem, which we solve using a spatial Branch-and-Bound algorithm for Global Optimization. The crucial step, i.e. the determination of the lower bound at each search tree node, relies on a sequence of reformulation steps which aim to linearize and relax the problem, and then to tighten the bound (these reformulations are applicable to a considerably larger class of problems than the Hartree-Fock problem). Some preliminary computational results are presented to illustrate our approach.

A New Metaheuristic Algorithm for Cluster Analysis

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Cluster analysis is an important tool for data exploration and it has been applied in a wide variety of fields like engineering, economics, computer sciences, life and medical sciences, earth sciences and social sciences. The typical cluster analysis consists of four steps (i.e. feature selection or extraction, clustering algorithm design or selection, cluster validation and results interpretation) with feedback pathway. These steps are closely related to each other and affect the derived clusters. In this paper, a new metaheuristic algorithm is proposed for cluster analysis. This algorithm uses combinations of metaheuristic algorithms like Tabu Search, Genetic Algorithms and Ant Colony Optimization to both feature selection step and to clustering algorithm design step. The proposed algorithm has been applied with very good results to many data sets.

Keywords: Cluster analysis, Feature selection problem, Clustering algorithm design, Metaheuristic algorithms, Tabu search, Genetic algorithm, Ant colony optimization.

Improved Scatter Search for the Global Optimization of Computationally Expensive Dynamic Models

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The metaheuristic known as scatter search is a population-based optimization method that has recently been shown to yield promising outcomes for solving combinatorial and nonlinear optimization problems. The main idea of the method is to combine solution vectors that have proved effective in a variety of problem settings. In this paper, we develop a general purpose heuristic for a class of nonlinear optimization problems. The procedure is based on the scatter search methodology and treats the objective function evaluation as a black box, making the search algorithm context-independent.

Most optimization problems in the chemical and bio-chemical industries are highly nonlinear in either the objective function or the constraints. Moreover, they usually present differential-algebraic systems of constraints. In this type of problems, the evaluation of a solution, or even the feasibility test of a set of values for the decision variables, can be a time-consuming operation. In this context, the optimization should be carried out in order to reduce the number of solutions' examinations (i.e. in order to keep the final computation time under reasonable values).

We have developed and implemented an improved scatter search procedure in Matlab for this special class of difficult optimization problems. Our development goes beyond a simple exercise of applying scatter search to this class of problems, but presents innovative mechanisms to obtain a good balance between intensification and diversification in a short term search horizon. Further, a kriging-based prediction method has been coupled to the main optimization routine in order to discard the evaluation of solution vectors that are not likely to provide high quality function values. Computational comparisons with other recently developed methods considering a set of challenging benchmark problems favour the proposed metaheuristic.

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Analysis of Greedy Approximation with Non-submodular Potential Functions

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In recent work of Du et al, we introduced a new method which can analyze a large class of greedy approximations with non-submodular potential functions, including some long-standing heuristics for Steiner trees, connected dominating sets, and power-assignment in wireless networks. There exist many greedy approximations for various combinatorial optimization problems, such as set covering, Steiner tree, subset-interconnection designs, etc.. There are also many methods to analyze these in the literature. However, all of the previously known methods are suitable only for those greedy approximations with submodular potential functions.

Gradient-Based IAGO Strategy for the Global Optimization of Expensive-to-Evaluate Functions and Application to Intake-Port Design

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Keywords - expected improvement, Gaussian process, global optimization, Kriging, optimal design

1 Introduction

When optimizing an expensive-to-evaluate function *f*, it is a common approach to use a cheap approximation for this function, which can lead to significant savings over traditional methods. In this context, successful global optimization techniques are generally based on Gaussian processes and Kriging (Chilès and Delfiner [1999]), which provide a probabilistic framework to account for the uncertainty on the function approximation.

Most Kriging-based strategies proposed in the past few years (see, e.g., Jones [2001]) *implicitly* seek a likely value for a global optimizer, and then assume it to be a suitable location for the next evaluation of *f*. Yet, given the past evaluations, the most likely location of a global optimizer is not necessarily a good evaluation point to improve the accumulated knowledge on this location.

Based on these considerations, the informational approach to global optimization (IAGO) strategy recently proposed (Villemonteix et al. [2006]) evaluates *f* where the potential reduction of uncertainty on the minimizer is deemed to be the highest. The entropy of the global optimizer density is taken as the uncertainty measure, and this density is approximated using conditional simulations of the Gaussian process modeling *f*. This approach has two main advantages over classical Kriging-based methods such as the *Efficient Globa Optimization* algorithm (Jones et al. [1998]). First, it allows significant savings on the number of evaluations of *f*. Second, the result under the form of a probability distribution is particularly attractive.

This paper presents a new approach aimed at reducing the computational cost of the entropy estimation step in the IAGO strategy. It is based on an approximation of the density of the global optimizer that uses the prediction by Kriging of the gradient of the Gaussian process. This approach is introduced in Section 2, and Section 3 presents an application in the automotive industry, for which ten hours of computation are required per evaluation of the cost function.

2 Outline of the approach proposed

With no loss of generality, we shall consider a minimization problem. Let $f : X \to \mathbb{R}$ be the function to be minimized (with X the factor space, a bounded subset of $\mathbb{R}^d$), and let $\boldsymbol{x}^* \in X$ be a global minimizer of *f*.

Assume that f is a sample path of a second-order Gaussian random process F with covariance $k(.,.)$. Given the vector of past evaluations $\boldsymbol{f}_s = [f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n)]$ (a sample value of the random vector $\boldsymbol{F}_s = [F(\boldsymbol{x}_1), \ldots, F(\boldsymbol{x}_n)]$), the Kriging predictor of $f(\boldsymbol{x})$ *is* the conditional mean of $F(\boldsymbol{x})$

$$m_c(\boldsymbol{x}) = \mathbb{E}(F(\boldsymbol{x}) | \boldsymbol{F}_\mathbb{S} = \boldsymbol{f}_\mathbb{S}).$$

Since F is Gaussian, $m_c(\boldsymbol{x})$ is obtained as a linear combination of $f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n)$, and the prediction error ε is a zero-mean Gaussian process with covariance denoted by $k_c(.,.)$. In practice, confidence intervals for the prediction can be computed from the value of $k_c(\boldsymbol{x}, \boldsymbol{x})$ (see top of Figure 1).

Given the past evaluations, f is modeled by F_c, the *conditioned process,* defined as

$$F_c(\boldsymbol{x}) = m_c(\boldsymbol{x}) + \varepsilon(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \mathbb{X}.$$

The sample paths of this process interpolate the data, and the distribution of F_c is the posterior distributionof F given the already available data. F_c thus represents all the behaviors that are deemed possible for f given what has been observed so far. A global minimizer $\boldsymbol{x}^*$ of f can then be viewed as a sample value of the random variable $\boldsymbol{X}^*$ minimizing F_c. Accordingly, the probability distribution $p_{\boldsymbol{x}^*|\,f_\mathbb{S}}$ of $\boldsymbol{X}^*$ given the data, will be considered as the current solution of the optimization problem. It represents all of what has been learned and assumed about $\boldsymbol{x}^*$ (see bottom of Figure 1). For example, when no values of f are available $p_{\boldsymbol{x}^*|\,f_\mathbb{S}}$ is flat, whereas when f is known exactly $p_{\boldsymbol{x}^*|\,f_\mathbb{S}}$ is zero everywhere except at global minimizers.

A central point in the IAGO method is the evaluation of the conditional entropy of $\boldsymbol{X}^*$ given the data and a candidate evaluation point $\boldsymbol{x}$, denoted by

$$H(\boldsymbol{X}^* | \boldsymbol{F}_s = \boldsymbol{f}_s, F_c(x)).$$

This conditional entropy is minimized to choose the evaluation point x_{new} that potentially most reduces the spread of $p_{\boldsymbol{x}^*|\,f_\mathbb{S}}$. To simplify computation, we propose to replace the simulation-based estimation of $p_{\boldsymbol{x}^*|\,f_\mathbb{S}}$ described in Villemonteix et al. *[2006]* by an approximation written as

$$\hat{p}_{\boldsymbol{X}^*|\,\boldsymbol{f}_\mathbb{S}}(\boldsymbol{x}) = \frac{1}{Z} \int_{-\infty}^{T} p_{F_c(\boldsymbol{x}), \nabla F_c(\boldsymbol{x})}(u, \boldsymbol{0}) du, \qquad (1)$$

with Z a normalization constant, and $p_{F_c(\chi), \nabla F_x(\chi)}$ the joint density of $F_c(x)$ and the gradient ∇F_c of F_c at x. The principle of this approximation is to look for stationary points below a threshold T (i.e. points x such that $F_c(\boldsymbol{x}) < \mathrm{T}$ and $\nabla F_c(\boldsymbol{x}) = 0$), taken as the lowest value off obtained so far. As the IAGO search progresses, T decreases along with the number of stationary points below T. As a result, the probability for such points to be local minimizers of F_c increases, and the distribution of the local minimizers below T converges to the distribution of the global minimizer.

For all x, $p_{F_c(\chi), \nabla F_x(\chi)}$ (.,.) is evaluated using the Kriging-based method described in Vazquez and Walter *[2005]*. Equation (1) then provides us with an approximation of the density of the global minimizer (see bottom of Figure l), which, though different from the actual density, turns out to provide an approximation that is good enough to suggest relevant evaluation points for f while being considerably cheaper. Figure *2* compares the two estimates of the conditional entropy obtained using the approach described in Villemonteix et al. [2006] and the new approach advocated in this paper.

3 Example of application

An illustrative application in the automotive industry for our approach is the design of intake ports, engine components that convey the air/fuel mixture to the combustion chambers. The rough shape of a typical intake port is presented on Figure 3. The importance of this component lies in the flow it induces in the combustion chamber, which has a direct impact on both the performance and the pollutant emissions of the engine. To comply with the new emission standards (Euro V and Euro VI), while satisfying the ever increasing need for engine performance, the shape of intake ports has to be carefully optimized. Building prototypes for tests is however exceedingly expensive, and each flow simulation by finite-element methods takes about ten hours on generally available processors. These difficulties make the approach advocated here particularly attractive given the general will for reduction of length and costs associated with development. The budget for function evaluation (100 at most) must therefore be allocated parsimoniously to determine near optimal values for at least seven shape parameters.

Two often-conflicting objectives have to be maximized simultaneously, namely the flow rate and the turbulence (the latter is quantified by the value of *tumble,* a scalar). To deal with this bi-objective problem, we wish to determine the Pareto front, i.e., the set of non-dominated parameter vectors (a parameter vector is said to dominate another when it is better in terms of both objectives).

To extend our approach to such a problem, we proceed as in Knowles and Hughes [2005], and consider linear combinations of the objective functions accounting for different zones of the Pareto front. In this paper, the coefficients will be chosen to direct the search towards the most uncertain regions of the Pareto front.

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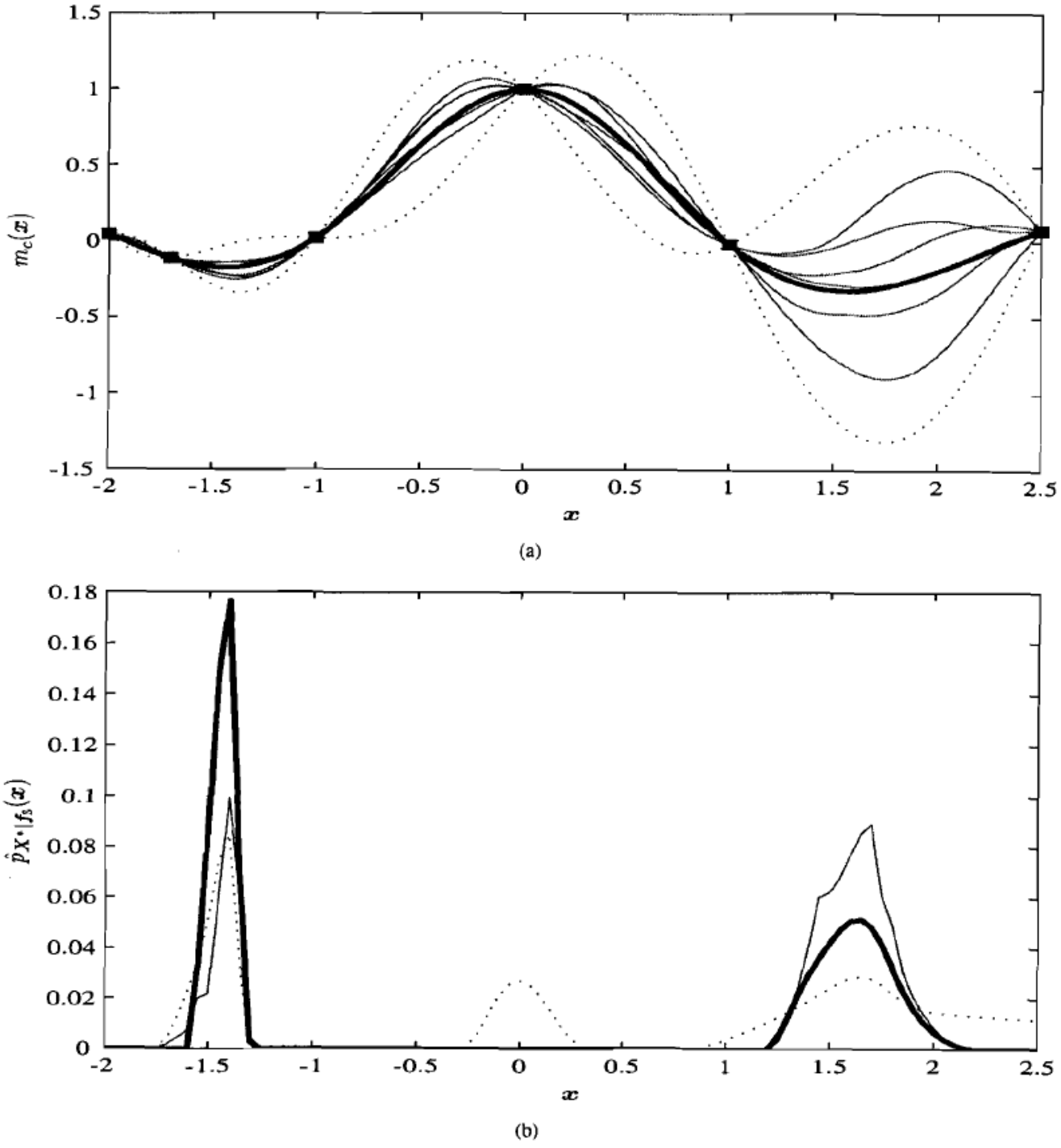

Figure 1: Evaluation of the conditional minimizer density associated with a Kriging prediction. Both simulation-based and derivative-based approximations are presented. [Top] Kriging prediction (bold line), based on a data sample (squares), and 95% confidence intervals. Conditional simulations are in thin lines). The histogram of the global minimizers of a sufficiently large set of these conditional simulations is used in Villemonteix et al. [2006] to approximate the density of the minimizer. [Bottom] Approximations of the minimizer density: with conditional simulations (thin line), and derivative-based (bold line). Although not identical, both approximations share the same support. The dotted line represents the probability density for the first derivative to be zero, i.e., $p_{\nabla F_c(\cdot)}(0)$.

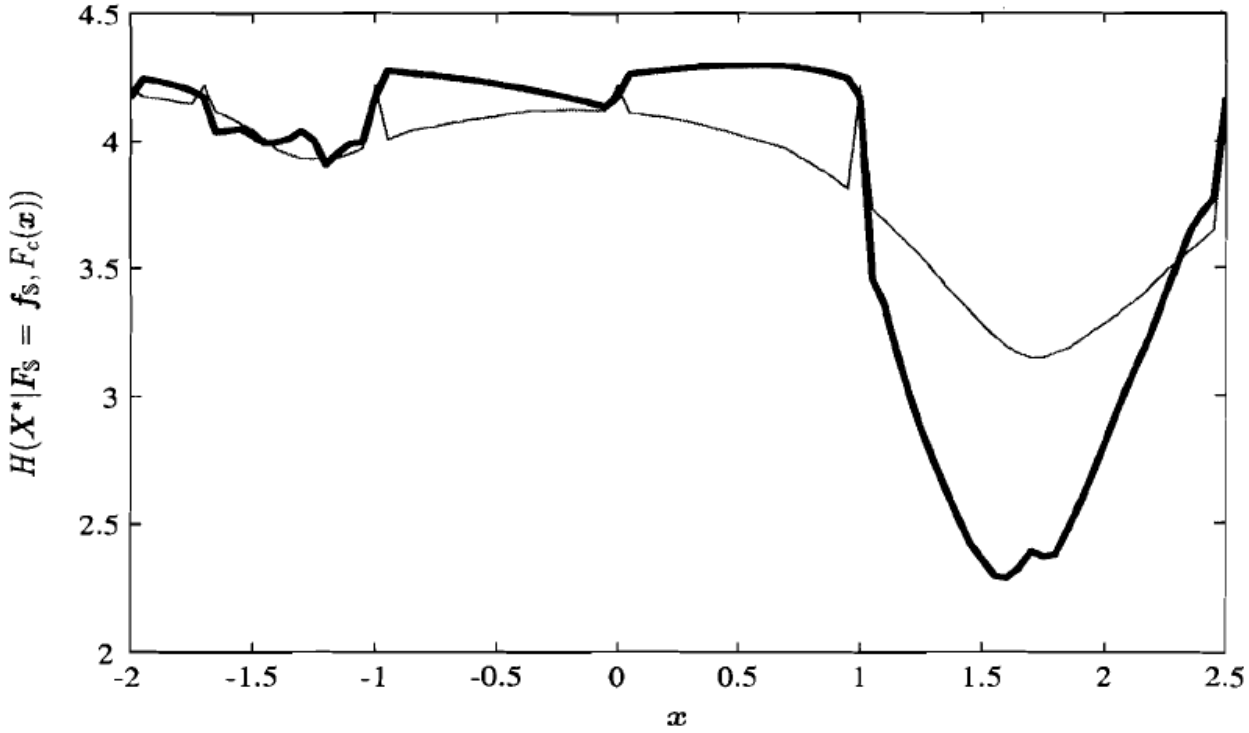

Figure 2: Criterion minimized for the choice of the next evaluation point given the data of figure 1. Thin line: as computed by the method described in Villemonteix et al. [2006] based on conditional simulations. Bold line: as computed using the approximations in (1).

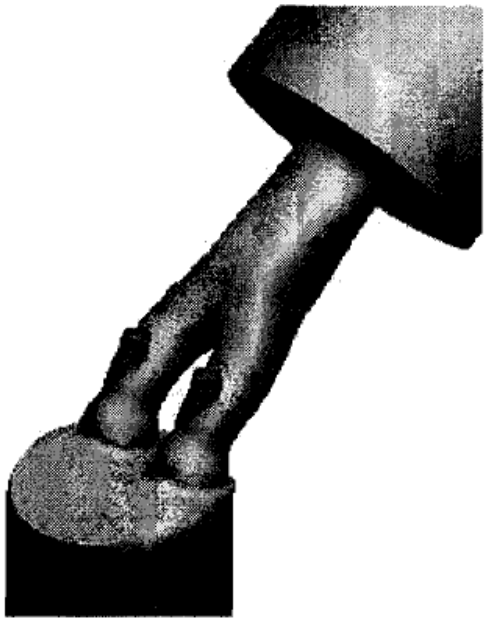

Figure 3: Intake port. The component itself is in the middle. Below is the combustion chamber. The upper cylinder is a tranquilizing volume necessary for the convergence of the finite-element simulations.

SDP versus RLT for Nonconvex QCQP

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We consider relaxations of nonconvex Quadratically Constrained Quadratic Programming (QCQP) based on combinations of the Reformulation-Linearization Technique (RLT) and Semidefinite Programming (SDP). From a theoretical standpoint we show that for each pair of variables, the addition of SDP constraints removes a substantial portion of the feasible region defined by RLT constraints alone. Computational experiments show that imposing both SDP and RLT constraints produces substantially tighter bounds than either technique alone. For geometric problems involving high degrees of symmetry we also show that additional symmetry-breaking constraints can have a substantial effect on both SDP and RLT bounds.

An Efficient Combined DCA and B&B using SDP Relaxation for Globally Solving Binary Quadratic Programs

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As optimization techniques are more and more widely used in engineering, economics and other sciences, an increasing number of problems arise from applications that cannot be globally solved by standard methods of linear and nonlinear programming. A part of these problems concerns binary quadratic programs, a special class of DC (Difference of Convex functions) programming, one of the most important domains in nonconvex programming.

The model of binary quadratic programming appears in diverse areas including economics, machine scheduling, solid-state physics, traffic message management, computer-aided design and location, facility location, Frequency Assignment, Register Allocation, Pattern Matching, Analysis of Biological and Archaeological Data, see [1, 3]. Many heuristic/deterministic methods have been developed in literature for its solution.

This paper investigates a new deterministic approach based on DC programming and DCA (DC Algorithm) for globally solving binary quadratic programs. An equivalent nonsmooth DC program, (i.e., minimization of a DC function on a convex set), is established by using exact penalty techniques in DC programming [14, 15], and solved by DCA.

Based on local optimality conditions and DC duality in DC programming, DCA was introduced by Pham Dinh Tao in 1985 as an extension of his earlier subgradient algorithms for concave programming, and extensively developed by Le Thi Hoai An and Pham Dinh Tao since 1994. The DCA has been successfully applied to real world nonconvex programs to which it quite often gave global solutions and proved to be more robust and more efficient than related standard methods, especially in large scale setting. It is, at the present time, one of the rare algorithms for nonsmooth nonconvex programming (see [8, 11, 12, 15]). To check globality of solutions computed by DCA, we propose a combination of DCA and Branch-and-Bound scheme (B&B) using SDP relaxation techniques [2, 16]. The combination, which aims at restarting DCA from new points generated by B&B with lower objective values, improves upper bounds and accelerates B&B.

Numerical simulations on several series of test problems show reliability and efficiency of DCA and the combined algorithm.

Keyword: DC programming, DC Algorithms (DCA), Nonconvex Quadratic Programming, Branch and Bound, SemiDefinite Programming.

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LaGO - Branch and Cut for Nonconvex MINLPs

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We present recent progress of the software package LaGO [4, 5] which is an implementation of an extended Branch and Cut algorithm for the solution of block-separable nonconvex mixed-integer nonlinear programs (MINLPs). LaGO does not require an algebraic formulation of the model, but only methods to evaluate function values and derivatives.

The algorithm reformulates every function into a block-separable form and computes convex envelopes for each term separately. For that purpose, nonquadratic functions are first replaced by quadratic underestimators using a powerful heuristic. Quadratic functions are then replaced by convex α-underestimators as introduced by Adjiman and Floudas [1].

Finally, a linear outer approximation is constructed by linearization of the convex relaxation and generation of mixed-integer rounding cuts [3]. Thus, the generation of these two kinds of cuts allows to inherit information about both nonlinearity in the functions and integrality restrictions.

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

Promising numerical results on medium size problems from the MINLPLib [2] show the efficiency of our method.

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Development of a Parallel Advanced Multidimensional Interval Analysis Tool for Global Optimization (PAMIGO)

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Interval methods for global optimisation use branch and bound (B&B) search strategies for an exhaustive search. In this way, they guarantee to enclose all minimiser solutions for a given precision. Basically the problem is subdivided into sub-problems until the solutions are found. Usually all the possible sub-problems are not evaluated because the B&B principle allows to discard many of them. B&B algorithms are suitable for parallel computation because sub-problems can be solved independently by different processors. AMIGO is an interval global optimisation algorithm which reduces the B&B search by a smart use of the objective function and its derivative values. This paper presents a parallel version of AMIGO (PAMIGO) for shared memory parallel computers.

Experiments were carried out on an Altix 3000 with 16 Itanium2 nodes and 64 Gb of RAM. However, the developed scheme is generic in the sense that it can be ported to nowadays personal computers with dual and quad core processors. This generic way of being implemented has been taken care of by basing the code of the algorithm on the concept of threads. Special care has been taken to dynamic load balancing, because the data structure is not known beforehand and dynamic. Experimental results show a promising speed-up and a corresponding execution time reduction for hard to solve problems on single uni-core processors.

Improvements on the GLOBAL Optimization Algorithm with Numerical Tests

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The talk considers the stochastic global optimization algorithm GLOBAL [3], as a non-derivative version of the method of Boender et al. [2]. We introduce a new Matlab based version of the original Fortran and C code together with some algorithmic improvements. The latter include a new, BFGS local search procedure, a new Matlab implementation of the UNIRANDI local search method [5], an extended capability for larger dimensional problems, and further changes to improve the efficiency of the procedure. A special attention has been devoted to increasing the reliability, and keeping the low computational complexity of the original implementation. The numerical test results will be discussed in detail, e.g.\ the comparison results with the old versions, with those of a new direct search procedure, C-GRASP [4], as well as on an extensive study regarding the scalability of the new method with respect of the dimension of the optimization problem. The first indicators are encouraging, and the new Matlab version of the algorithm GLOBAL should be available soon at the usual internet place (www.inf.u-szeged.hu/~csendes/reg/regform.php) for academic and nonprofit purposes. Some real life applications are also reported from the fields of chemical engineering and control [1, 6, 7].

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Learning the Best Combination of Solvers in a Distributed Global Optimization Environment

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A generic distributed computing environment built for the internal network of the European Space Agency has been developed [1] and used to distribute different global optimization techniques. Differential Evolution, Particle Swarm Optimization, Genetic Algorithm and Simulated Annealing algorithms have been implemented and tested to show the functionality of the environment. In this paper a distributed global multi-objective optimizer is introduced which is able to learn and apply the best combination of the available solving strategies when tackling a generic black-box problems. A set of heuristics is developed and investigated to employ the available solvers in an intelligent and co-operative way. The efficiency is demonstrated on a large collection of standard test problems as well as some difficult global optimization problems arising in space mission analysis.

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