3rd International Conference on Optimization Methods and Software 2012

May 13th – May 17th, 2012

Chania, Crete, Greece

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Plenary talks

Enforcing convergence to all members of the Broyden family of methods for unconstrained optimization

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The Broyden family of quasi-Newton methods for unconstrained optimization will be considered. It is well-known that if a member of this family is defined sufficiently close to the robust BFGS method, then useful convergence properties are usually obtained. These properties will be extended to other members of the family provided that the updating parameter satisfies certain conditions based on some estimation of the size of the eigenvalues of Hessian approximations. These conditions are satisfied for all members of the family near the solution of any convex optimization problem. Otherwise, when the iterate is remote away from the solution, they are simply enforced. Numerical results will be described.

Second-order optimality conditions and shooting algorithms for optimal control problems

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We will discuss the second-order optimality conditions, both necessary and sufficient, for optimal control problems of ODEs with control and state constraints, for weak and strong solutions. In the second case the second-order optimality conditions typically involve Pontryagin multipliers. We will show the close link with the well-posedness of the shooting algorithm in various settings, and with the analysis of discretization errors.

Libraries of algorithms for solving large-scale LP problem and for global optimization

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LP projection method is used for finding normal solution of LP problem. This approach is close to the quadratic penalty function method and to the modified Langrangian function method. This method yields the exact projection of a given point on the solution set of primal LP problem as a result of the single unconstrained maximization of an auxiliary piecewise quadratic concave function for any sufficiently large values of the penalty parameter. A generalized Newton method with a stepsize chosen using Armijo's rule was used for unconstrained maximization. The proof of globally convergent finitely terminating generalized Newton method for piecewise quadratic function was giving. LP projection method solves LP problems with a very large ($\sim 10^7$) number of variables and moderate ($\sim 10^5$) number of constraints. In a similar way, the exact projection of a given point on the solution set of the dual LP problem can be obtained by nonnegative constrained maximization of auxiliary quadratic function for sufficiently large but finite values of the penalty parameter. A library of algorithms for global optimization was developed on the basis of nonuniform space covering technique which was proposed by author in 1971 for Lipshitzian functions. Later this approach was generalized and was applied to nonlinear programming problem and to multiobjective optimization. The objective and constraints functions may contain both continuous and integer variables and the objective may be non-convex and multiextremal. The covering algorithm for multiobjective optimization has been implemented in the BNB-Solver framework. The BNB-Solver is a generic framework for implementing optimization algorithms on serial and parallel computers.

Computational experiments for various test problems demonstrated that this algorithm reliably constructed the ϵ-Pareto set approximations in a reasonable time. Obtained approximations provide uniform covering of the Pareto-set.

Smoothing approach to equilibrium problems with shared complementarity constraints

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The equilibrium problem with equilibrium constraints (EPEC) can be looked on as a generalization of Nash equilibrium problem (NEP) and the mathematical program with equilibrium constraints (MPEC). In this paper, we particularly consider a special class of EPECs where a common parametric P-matrix linear complementarity system is contained in all players' strategy sets. After reformulating the EPEC as an equivalent nonsmooth NEP, we use a smoothing method to construct a sequence of smoothed NEPs that approximate the original problem. We consider two solution concepts, global Nash equilibrium and stationary Nash equilibrium, and establish some results about the convergence of approximate Nash equilibria. Moreover we show some illustrative numerical examples.

(Joint work with Ming Hu.)

Cubic overestimation and secant updating for unconstrained optimization

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The discrepancy between an objective function f and its local quadratic model $f(x) + g(x)^T s + sH(x)s/2 \approx f(x + s)$ at the current iterate x is estimated using a *cubic* term $q\|s\|^3/3$. Potential steps are chosen such that they minimize the overestimating function $g(x)^\top s + s^\top Bs/2 + q\|s\|^3/3$ with $B \approx H(x)$. This ensures $f(x + s) < f(x)$ unless B differs significantly from $H(x)$ or the scalar $q > 0$ is too small. Either or both quantities are updated over unsuccessful and successful steps alike. For an algorithm employing both the symmetric rank one update and the BFGS formula we show that either $\inf \|g\| = 0$ or $\sup \|B\| = \infty$, provided the Hessian $H(x)$ is locally Lipschitz on R^n.

MPECs in function space

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Several classes of mathematical programs with equilibrium constraints (MPECs), which are posed in function space and which are related to the optimal control of (partial differential) variational inequalities will be considered. Based on set-valued analysis tools suitable stationarity principles will be derived. Particular focus will be put on constraints on the gradient of the state as well as on upper level control constraints. Several extensions of the framework are discussed and a solution algorithm along with numerical results will be presented.

Domain decomposition techniques in topology optimization

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Recent advances in the application of domain decomposition techniques to topology optimization of mechanical structures will be presented. The topology optimization problem can be modelled as a (very-)large-scale convex constrained optimization problem. The large dimensionality stems from very fine discretization by finite elements. We will present several ways how to use domain decomposition techniques, known from the solution of linear systems, to solve large instances of the problem.

(Joint work with M. Kojima (Tokyo), D. Loghin and J. Turner (Birmingham).)

Subgradient methods for huge-scale optimization problems

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We consider a new class of huge-scale problems, the problems with sparse subgradients. The most important functions of this type are piece-wise linear. For optimization problems with uniform sparsity of corresponding linear operators, we suggest a very efficient implementation of subgradient iterations, which total cost depends logarithmically in the dimension. This technique is based on a recursive update of the results of matrix/vector products and the values of symmetric functions. It works well, for example, for matrices with few nonzero diagonals and for max-type functions.

We show that the updating technique can be efficiently coupled with the simplest subgradient methods, the unconstrained minimization method by B.Polyak, and the constrained minimization scheme by N.Shor. Similar results can be obtained for a new nonsmooth random variant of a coordinate descent scheme. We present also the promising results of preliminary computational experiments.

Detecting critical subsets (nodes, edges, shortest paths, or cliques) in large networks

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In network analysis, the problem of detecting subsets of elements important to the connectivity of a network (i.e., critical elements) has become a fundamental task over the last few years. Identifying the nodes, arcs, paths, clusters, cliques, etc., that are responsible for network cohesion can be crucial for studying many fundamental properties of a network. Depending on the context, finding these elements can help to analyze structural characteristics such as, attack tolerance, robustness, and vulnerability. Furthermore we can classify critical elements based on their centrality, prestige, reputation and can determine dominant clusters and partitions. From the point of view of robustness and vulnerability analysis, evaluating how well a network will perform under certain disruptive events plays a vital role in the design and operation of such a network. To detect vulnerability issues, it is of particular importance to analyze how well connected a network will remain after a disruptive event takes place, destroying or impairing a set of its elements. The main goal is to identify the set of critical elements that must be protected or reinforced in order to mitigate the negative impact that the absence of such elements may produce in the network. Applications are typically found in homeland security, energy grid, evacuation planning, immunization strategies, financial networks, biological networks, and transportation. From the member-classification perspective, identifying members with a high reputation and influential power within a social network could be of great importance when designing a marketing strategy.

Positioning a product, spreading a rumor, or developing a campaign against drugs and alcohol abuse may have a great impact over society if the strategy is properly targeted among the most influential and recognized members of a community. The recent emergence of social networks such as Facebook, Twitter, LinkedIn, etc. provide countless applications for problems of critical-element detection. In addition, determining dominant cliques or clusters over different industries and markets via critical clique detection may be crucial in the analysis of market share concentrations and debt concentrations, spotting possible collusive actions or even helping to prevent future economic crises. This presentation surveys some of the recent advances for solving these kinds of problems including heuristics, mathematical programing, dynamic programing, approximation algorithms, and simulation approaches. We also summarize some applications that can be found in the literature and present further motivation for the use of these methodologies for network analysis in a broader context.

(Joint work with Steffen Rebennack, Ashwin Arulselvan, Clayton Commander, Vladimir Boginski, Chrysafis Vogiatzis, Jose L. Walteros, Neng Fan, Donatella Granata, and Olga Khvostova.)

Linearly constrained optimization without derivatives

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The author has supplied the NEWUOA and BOBYQA packages for optimization without derivatives, when there are no constraints and simple bounds on the variables, respectively. They employ trust regions, quadratic models, and the symmetric Broyden method for updating the second derivatives of the models. They have calculated the solutions of many problems to high accuracy, even when the number of variables, n say, is in the hundreds. Further, when n is large, the total number of evaluations of the objective function seems to be about a multiple of n, instead of being of magnitude n squared. At present the author is trying to develop an extension of these packages that allows general linear constraints on the variables. In order to construct good models in the full space of the variables, it is assumed that the objective function can be calculated at infeasible points, but trust region steps have to satisfy the constraints. The techniques that are under consideration will be described, including a version of truncated conjugate gradients for efficiency when n is large. The progress so far will be reported, but the conference may be too soon for numerical results.

Complex optimization in quantum physics

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In the study of the quantum entanglement problem, there are optimization problems involving complex variables. In this talk, we will analyze such optimization problems and report the result on the minimum Hartree value.

Alternating linearization for structured regularization problems

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We adapt the alternating linearization method for proximal decomposition to structured regularization problems, in particular, to the generalized lasso problems. The method is related to two well-known operator splitting methods, the Douglas–Rachford and the Peaceman–Rachford method, but it has descent properties with respect to the objective function. Its convergence mechanism is related to that of bundle methods of nonsmooth optimization. We also discuss implementation for very large problems, with the use of specialized algorithms and sparse data structures. Finally, we present numerical results for several synthetic and real-world examples, including a three-dimensional fused lasso problem, which illustrate the scalability, efficacy, and accuracy of the method.

Preconditioning techniques for optimization with PDEs

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We review recent progress in the numerical solution of optimization problems with partial differential equations as constraints. Preconditioning the Karush-Kuhn-Tucker system in the solution of the necessary optimality system is an important task. We show research efforts in this field during the past years with special emphasis to the role of Bramble-Pasciak preconditioners. We conclude with remarks on the impact of the original nonlinear structure of the problem on preconditioning techniques.

Inexact decomposition methods for constrained convex optimization problems and application to network equilibrium problems

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In this work we propose convergent inexact decomposition methods for smooth problems defined on the Cartesian product of convex sets. More specifically, we present a conceptual model of decomposition algorithm using a restriction of the feasible sets (in order to possibly exploiting column generation strategies), and gradient projection mappings (for computing inexact solutions of the generated subproblems). The global convergence of the algorithm is proved under suitable assumptions on the restriction of the feasible sets. Due to the generality of the assumptions stated, the proposed algorithm model can be the framework to develop decomposition algorithms for different classes of problems. In the talk we focus on the class of network equilibrium problems, we present convergent decomposition schemes derived from the algorithm model, and we show computational results obtained on medium-large dimensional problems.

The cubic regularization algorithm and recent complexity issues for nonconvex optimization

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The talk will survey recent developments in the analysis of worst-case complexity bounds for algorithms intended for solving nonconvex continuous optimization problems. The convergence to first- and second-order critical points in the unconstrained case will be considered first, and methods such as steepest descent, Newton and several of its variants will be revisited. The talk will also present some approaches for the constrained case. Some relatively surprising results will be given and the special nature of the cubic regularization method (ARC) will be pointed out.

Multilevel methods for PDE-constrained optimization involving adaptive discretizations and reduced order models

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We consider optimization problems governed by time-dependentpartial differential equations. Multilevel techniques use a hierarchyof approximations to this infinite dimensional problem and offerthe potential to carry out most optimization iterations on comparablycoarse discretizations.In this talk we discuss the efficient interplay between the optimizationmethod, adaptive discretizations of the PDE, reduced order models derivedfrom these discretizations, and error estimators.To this end, we describe an adaptive multilevel SQP method that generatesa hierarchy of adaptive discretizations during the optimizationiteration using adaptive finite-element approximations and reducedorder models such as POD. The adaptive refinement strategy is basedon a posteriori error estimators for the PDE-constraint, the adjointequation and the criticality measure. The resulting optimization methodsallows to use existing adaptive PDE-solvers and error estimators in amodular way.We demonstrate the efficiency of the approach by numerical examples.

Sparse Hessian recovery and trust-region methods based on probabilistic models

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In many application problems in optimization, one has little or no correlation between problem variables, and such (sparsity) structure is unknown in advance when optimizing without derivatives. We will show that quadratic interpolation models computed by l1-minimization recover the Hessian sparsity of the function being modeled, when using random sample sets. Given a considerable level of sparsity in the unknown Hessian of the function, such models can achieve the accuracy of second order Taylor ones with a number of sample points (or observations) significantly lower than $O(n^2)$.

The use of such modeling techniques in derivative-free optimization led us to the consideration of trust-region methods where the accuracy of the models is given with some positive probability. We will show that as long as such probability of model accuracy is over $1/2$, one can ensure, almost surely, some form of convergence to first and second order stationary points.

The simplex and policy-iteration methods are strongly polynomial for the Markov decision problem with a constant discount factor

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We prove that the classic policy-iteration method (Howard 1960), including the Simplex method (Dantzig 1947) with the most-negative-reduced-cost pivoting rule, is a strongly polynomial-time algorithm for solving the Markov decision problem (MDP) with a constant discount factor. Furthermore, the computational complexity of the policy-iteration method (including the Simplex method) is superior to that of the only known strongly polynomial-time interior-point algorithm for solving this problem. The result is surprising since the Simplex method with the same pivoting rule was shown to be exponential for solving a general linear programming (LP) problem, the Simplex (or simple policy-iteration) method with the smallest-index pivoting rule was shown to be exponential for solving an MDP regardless of discount rates, and the policy-iteration method was recently shown to be exponential for solving a undiscounted MDP. We also extend the result to solving MDPs with sub-stochastic and transient state transition probability matrices.

The Frank-Wolfe algorithm, away steps, and core sets in optimization

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Recently, many studies have centered around developing algorithms for large-scale optimization problems by identifying a small subset of the constraints and/or variables and solving the resulting smaller optimization problem instead. Such small subsets are known as *core sets*. For a certain class of optimization problems, one can explicitly compute such a small subset with the property that the resulting optimal solution is a close approximation of the optimal solution of the original problem. Such problems mainly include geometric optimization problems such as minimum containment, clustering, and classifcation. In this talk, we discuss the connections between core sets and the Frank-Wolfe algorithm and its variants. In particular, we discuss how the Frank-Wolfe algorithm forms a basis for the existence of small core sets for various large-scale optimization problems.

Hybrid algorithm for power maximization interference alignment problem of MIMO channels

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Considering a K-user MIMO interference channel, we present a desired signal power maximization model with interference alignment (IA) conditions as constraints to design proper users' precoders and decoders, which forms a complex matrix optimization problem. Courant penalty function technique is applied to combine the leakage interference and the desired signal power as the new objective function. We propose an $e\pm$client hybrid algorithm to solve the problem, which includes two parts. As the first part, a new algorithm iterates with Householder transformation to preserve the orthogonality of precoders and decoders. In each iteration, the matrix optimization problem is decomposed to several one dimensional optimization problems. From any initial point, this algorithm can obtain precoders and decoders with low leakage interference in short time. In the second part, an alternating minimization algorithm with Courant penalty function technique is proposed to perfectly align the interference from the output point of the first part. Analysis shows that generally the hybrid algorithm has lower computational complexity than the existed maximum signal power (MSP) algorithm. Simulations reveal that the hybrid algorithm achieves similar performance as MSP algorithm with less computing time, and shows better performance than the conventional IA algorithm in terms of sum rate.

Contributed talks

Transformations of proper edge colorings of graphs and their application in scheduling

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An edge t-coloring of a graph G is an assignment of the colors $1, 2, ..., t$ to the edges of G, one color to each edge. Such a coloring is called proper if no pair of adjacent edges receive the same color.

Graph coloring theory has one of central positions in discrete mathematics. It appears in many places with seemingly no or little connections to coloring. For example, many problems on school timetables can be formulated in terms of edge colorings of bipartite graphs.

Consider also another example: Given a telecommunication network, we have to schedule file transfers in the network, each file engaging two corresponding nodes: sender and receiver simultaneously. It is necessary to minimize the average response time, or equivalently to minimize the sum of the transfers completion times.

In terms of graph theory this problem can be reformulated in the following way: Find a proper edge coloring of the corresponding graph G where the sum of assigned colors of all edges of G is minimized.

We discuss the following problem: Let $L_t(G)$ be the set of all proper edge colorings of a graph G with colors $1, 2, ..., t$. Find a system S of transformations such that for any $f, g \in L_t(G)$ there exists a sequence $f_1, ..., f_k$ of proper edge colorings in $L_t(G)$, $k = k(f, g) \geq 2$, where $f_1 = f$, $f_k = g$ and f_{i+1} is obtained from f_i by one of the transformations in S, $i = 1, ..., k-1$. Such a system is called a complete system of transformations for $L_t(G)$.

Complete system of transformations can be very useful in scheduling problems which are formulated as proper edge coloring problems. In order to find an optimal schedule (optimal coloring) we can begin by finding any proper coloring of G, and then use our transformations to make the solution a better and better approximation to the optimal solution.

Tolerance Based Algorithms for the Asymmetric Capacitated VRP

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In this paper we develop a tolerance-based Branch-and-Bound algorithm for solving the Asymmetric Capacitated Vehicle Routing Problem (ACVRP). Our main contributions are represented by the tolerance based lower bound and branching rule including a preliminary clustering of all customers into p clusters (routes) by means of solving the corresponding p-median problem either approximately or exactly. Computational experiments with different testbeds are reported.

(Joint work with Boris Goldengorin, Evgeny Maslov, Panos M. Pardalos.)

Monotonicity recovering optimization methods for postprocessing finite element solutions

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Partially lost monotonicity of the numerical solution is a typical drawback of the conventional methods of approximation, such as finite elements (FE), finite volumes, and mixed finite elements. The problem of monotonicity is particularly important in cases of highly anisotropic diffusion tensors or distorted unstructured meshes. Another drawback of the conventional methods is a possible violation of the discrete maximum principle, which establishes lower and upper bounds for the solution.

In this talk, we suggest a least-change correction to available finite element (FE) solution. This postprocessing procedure is aimed on recovering the monotonicity and some other important properties that may not be exhibited by the FE solution. It is based on solving a monotonic regression problem with some extra constraints. One of them is a linear equality-type constraint which models the conservativity requirement. The other ones are box-type constraints, and they originate from the discrete maximum principle. The resulting postprocessing problem is a large scale convex quadratic optimization problem. We show that the postprocessed FE solution preserves the accuracy of the discrete FE approximation.

We present an algorithm for solving the postprocessing problem. It can be viewed as a dual ascent method based on the Lagrangian relaxation of the equality constraint. Its efficiency is demonstrated by the results of numerical experiments.

(Joint work with Ivan Kapyrin and Yuri Vassilevski, Institute of Numerical Mathematics Russian Academy of Sciences, Moscow, Russia)

Pattern-based approach to the cell formation problem

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In this paper we introduce the notion of a "pattern" in the Linear Assignment Problem (LAP) and show that patterns might be useful as an improvement heuristic for the Cell Formation Problem (CFP) in Group Technology. We define a "pattern" as a specific collection of cells in the given machines-parts input matrix reflecting a block-diagonal structure of a feasible solution to the CFP. We further reduce the CFP to a sequence of LAPs within which we solve each LAP at the first step w.r.t. the best rows (machines) permutation r. At the second step we use the permuted machines-parts matrix by means of an optimal permutation r as an input machines-parts matrix and solve the corresponding LAP w.r.t. the columns (parts) with an optimal permutation c. We summarize our approach by means of a computational study applied to the well known large-sized benchmark CFP instances.

(Joint work with Mikhail Batsyn, Boris Goldengorin, Evgeny Maslov, Panos M. Pardalos)

On the evaluation complexity of cubic regularization methods for potentially rank-deficient nonlinear least-squares problems and its relevance to constrained nonlinear optimization

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We propose a new termination criteria suitable for potentially singular, zero or non-zero residual, least-squares problems, with which cubic regularization variants take at most $\mathcal{O}(\epsilon^{-3/2})$ residual- and Jacobian-evaluations to drive either the Euclidean norm of the residual or its gradient below ϵ; this is the best-known bound for potentially rank-deficient nonlinear least-squares problems. We then apply the new optimality measure and cubic regularization steps to a family of least-squares merit functions in the context of a target-following algorithm for nonlinear equality-constrained problems; this approach yields the first evaluation complexity bound of order $\epsilon^{-3/2}$ for nonconvexly constrained problems when higher accuracy is required for primal feasibility than for dual first-order criticality.

(Joint with Nick Gould and Philippe Toint)

Global tolerances in combinatorial optimization with an additive objective function

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The currently adopted notion of a tolerance in combinatorial optimization is defined referring to an arbitrarily chosen optimal solution, i.e., locally. In this talk we introduce global tolerances with respect to the set of all optimal solutions, and show that the assumption of nonembededdness of the set of feasible solutions in the provided relations between the extremal values of upper and lower global tolerances can be relaxed.

(Joint work with Boris Goldengorin and Panos M. Pardalos)

A BBCG method for unconstrained optimization

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A new method is proposed for unconstrained optimization. At the initial stage, since the objective function is generally nonlinear, the method performs similarly to the Barzilai-Borwein (BB) gradient method. When the objective function is close to be quadratic, the method then performs as the conjugate gradient (CG) method. Consequently, we call the method by BBCG. Some analysis is also given for the BBCG method.

A stochastic zonal decomposition algorithm for network energy management problems

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We consider a network with zones and links. Each zone has its own production units and is subject to a unit commitment problem: it has to satisfy a stochastic demand using its hydro and thermal units and eventually importing and exporting using its links. Assuming that we have the appropriate tools to solve a single unit commitment problem (approximate dynamic programming, SDDP, etc.), the proposed algorithm allows us to coordinate the productions of all zones. The proposed algorithm is a stochastic forward-backward splitting algorithm close to quantity decomposition algorithms. After presenting the problem and the algorithm in a deterministic framework, we present an extension to solve stochastic optimal control problems with a network structure. Then, a numerical application will be presented to solve a coordinated European energy management problem.

Piecewise monotonic approximation: Applications to signal restoration

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This paper discusses, in the context of signal restoration, image processing and inversion, areas where piecewise monotonic approximation (pma) algorithms have found important applications. The pma method originated by M. J. D. Powell, while some highly efficient algorithms have been studied and developed by Powell, the author and associates. To be specific, given n measurements of a univariate function, which have been altered by random errors, this method minimizes the sum of the squares of the errors by requiring k monotonic sections, alternately increasing and decreasing, where the positions of the turning points are integer variables of the minimization calculation. Although the problem can have n over k local minima, the algorithms calculate a global solution within a fraction of quadratic complexity in n. This is very desirable in fMRI, because, for example, an image matrix is composed of at least 256 rows times 3584 vectors and pma has to be employed on each of the rows throughout the image. Moreover, besides noise reduction and automatic calculation of the turning points, pma controls noise ringing unlike low-pass-filter-type smoothing and prevents effects resulting from the spurious wavelet extrema in signal restoration.

Decomposition methods for two-stage problems with stochastic order constraints

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We consider two-stage risk-averse stochastic optimization problems with a stochastic ordering constraint on the recourse function. Two stochastic orders are discussed: first order stochastic dominance and the increasing convex order. Two new characterizations of the increasing convex order relation are provided. They are based on conditional expectations and on integrated quantile function representing a counterpart of the Lorenz function. We propose new decomposition methods to solve the problems and prove their convergence. Our methods exploit the decomposition structure of the risk-neutral two-stage problems and construct successive approximations of the stochastic ordering constraints. Numerical results confirm the efficiency of the methods.

On the shortest path problem with negative cost cycles

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In this work, the elementary single-source all-destinations shortest path problem is considered. Given a directed graph, containing negative cost cycles, the aim is to find the paths with minimum cost from a source node to each other node, that do not contain repeated nodes. Three different solution strategies are proposed to solve the problem under investigation and their theoretical properties are investigated. The proposed solution approaches are based on the idea to compute for each node the minimum set of paths such that the elementary shortest path is found for all nodes. The first is a dynamic programming approach that uses dummy node resources in order to avoid cycles in the optimal solution. The proposed approach can be viewed as a modified version of the solution strategies defined to solve the Resource Constrained Elementary Shortest Path Problem (RCESPP). It is worth observing that it is not possible to apply directly solution approaches for the RCESPP to solve the elementary single-source all-destinations shortest path problem. A multi-dimensional labeling procedure is devised and the dimension of the label is updated dynamically. The second method is based on the solution of the k shortest paths problem, where k is considered as a variable that can take different values for each node. The algorithm iteratively increments the value of k associated with a specific node. The main idea is to determine the smallest value of k for each node such that the elementary shortest path is found for all nodes. The last solution strategy is an enumerative approach based on a tree structure, constructed with a cycle elimination rule. This work represents the first attempt to study and to propose solution approaches in order to optimally solve the shortest path problem in presence of negative cost cycles.

The main aim is to give ideas on how to solve the single-source all-destinations version of the problem and theoretical aspects related to the innovative proposed strategies to solve the problem at hand are shown.

(Joint work with Francesca Guerriero.)

A coupled monotonic regression problem

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The following problem arises in experimental psychology. Levels of performance on two tests are obtained under n different conditions, defined by the orthogonal combination of 2 or more independent variables. Two hypotheses are proposed.

H1: That the effects of the independent variables are mediated by a single latent variable (e.g., a psychological process of some sort); and

H2: That the effects are mediated by more than one latent variable.

Under H2, it is assumed we know enough about the effects of the independent variables to impose a common partial order on the two dependent variables across the n conditions. To fit this model is to solve the following extension of a standard monotonic regression (MR) problem: Let $a, b \in R^n$ be vectors of observed values and let $v, w \in R^n$ be vectors of positive weights and let E be a set of edges on a directed graph $G(N, E)$, for $N = \{1, 2, ..., n\}$, that defines a partial order. Now find vectors, $x^*, y^* \in R^n$, that solve:

$$\min \sum_{i=0}^{n} ((v_i(x_i - a_i)^2 + w_i(y_i - b_i)^2)$$
$$s.t. \quad x_i \leq x_j, y_i \leq y_j, \forall (i, j) \in E.$$

Under H1, as well as assuming the same partial order, it is further assumed that x and y are monotonic functions of the common latent variable. This requires that,

$$x_i < x_j \implies y_i \leq y_j, \forall i, j \in N$$
$$y_i < y_j \implies x_i \leq x_j, \forall i, j \in N.$$

To fit this model is to solve the following non-standard MR problem:

Let $L(E)$ be the set of linear extensions of the partial order defined by E. Find vectors, $x^*, y^* \in \mathbb{R}^n$ and $T \in L(E)$ that solve:

$$\min \sum_{i=0}^{n} ((v_i(x_i - a_i)^2 + w_i(y_i - b_i)^2), s.t. \quad x_i \leq x_j, y_i \leq y_j, \forall (i,j) \in T.$$

We describe a novel branch and bound algorithm for this problem.

(Joint work with Oleg Burdakov and Mike Kalish.)

Optimal design and operation of transmission gas pipelines

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Natural gas is increasingly being used as an energy source. Natural gas transmission pipelines transport large quantities of natural gas across long distances. They operate at high pressures and utilize a series of compressor stations at frequent intervals along the pipeline (more than 60 miles) to move the gas over long distances.

The objective function is given by a nonlinear function of flow rates and pressures. The optimization problem has been solved with number of decision variables and the number of constraints to find the optimal design variables and operations of transmission pipelines over flat terrain. The objective function is included installation cost of pipelines, compressor stations, fuel consumption in compressor stations, maintenance, labor and supervision. The software computer program Lingo is used to obtain the solution procedure for optimal design and operation of transmission gas pipelines.

Barrier methods for critical exponent problems in general relativity

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The Einstein field equations for general relativity describe how gravity interacts with matter and energy. The equations are a system of ten coupled equations, comprised of six evolution equations and four constraint equations. The constraint equations must be enforced at each time step when solving the evolution equations. Implicit in the Einstein constraint equations is an additional simple inequality. We look at solving these equations using barrier methods together with a traditional finite element approach.

Automated derivation of the discrete adjoint of high-level transient finite element programs

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In this paper we demonstrate the capability of automatically deriving the associated discrete adjoint and tangent linear models from a forward model written in a high-level finite element computing environment.

High-level systems allow the developer to express the variational form to be solved in near-mathematical notation, from which the low-level code is automatically generated by a custom finite element compiler. These high-level systems have a key advantage: because the mathematical structure of the problem to be solved is preserved, they are much more amenable to automated analysis and manipulation than a low-level code written in a language such as C or Fortran.

We present a software package capable of automatically deriving adjoint and tangent linear models from forward models written in the DOLFIN finite element computing environment. The approach relies on run-time annotation of the temporal structure of the model, and employs the same finite element form compiler to automatically generate the assembly code for the derived models. This method requires only trivial changes to most forward models, and works even for complex time-dependent nonlinear forward models.

Many of the difficulties of AD are caused by the necessity of dealing with the low-level implementation details of the model code. By contrast, by adopting this high-level abstraction, many of these issues simply disappear.

For example, both the adjoint and tangent linear models work in parallel, with no particular parallel support required by the tool which derives them. The adjoint model employs checkpointing schemes to mitigate storage requirements for nonlinear models, without the additional annotation usually necessary in the AD case. The adjoint and tangent linear models work even when complex solution strategies such as matrix-free solvers are used. The efficiency and generality of the approach are demonstrated with examples from several different scientific applications.

Matrix-free interior point method for compressed sensing problems

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We consider a class of optimization problems for sparse signal reconstruction which arise in the field of Compressed Sensing. A plethora of approaches and solvers exist for such problems, for example GPSR, FPC AS, SPGL1, NestA, l1ls, PDCO to mention a few.

Compressed Sensing applications lead to very well conditioned optimization problems and therefore can be solved easily by simple first-order methods. Unspecialized second-order methods also have been applied although without being competitive enough. In this work we demonstrate that a second-order method such as an interior point algorithm can be specialized for the CS problems and offer a competitive alternative to the existing approaches. The new approach is based on the Matrix-free Interior Point Method [1] in which an iterative (Krylov-subspace) method is employed to compute an inexact Newton direction. The matrix-free IPM does not require an explicit storage of the constraint matrix but accesses it only to get the matrix-vector products. It is therefore well-suited for solving large scale problems because it can take full advantage of the low-complexity fast matrix-vector operations. An approximated partial Cholesky preconditioner of rank one is employed to accelerate the convergence of the Krylov-subspace method. Additionally, suitable approximation of the diagonal of the normal equations system matrix is performed, required by the Cholesky decomposition process, which further reduces the computational effort. The computation of the preconditioner requires only matrix-vector products and fits into the matrix-free regime.

The convergence of the proposed IPM scheme in just a few iterations (7-15 iterations) for large scale one-dimensional signals (vector of length 1 million) confirms that the new approach is efficient and compares favourably with other state-of-the-art solvers.

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Coordinate search algorithms in multigrid optimization

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Optimization problems arising from the discretization of continuous problems are frequently encountered in many applications. Typical examples can be found in the contexts of PDE constrained optimization, optimal control, calculus of variations and image reconstruction (Nash, 2000), (Nash and Lewis, 2005), (Gratton et al., 2010). Supposing the problem can be discretized according to some grid parameter, one can define a hierarchy of problems ordered from coarsest to finest. It has been shown that in such cases multilevel methods, directly inspired by classical multigrid methods for linear and non-linear systems, provide an extremely effective tool to find a solution on the finest grid.

A number of such schemes has recently appeared in literature for both unconstrained and constrained optimization problems (Nash, 2000, 2010), (Gratton et al., 2008, 2010). Broadly speaking, they consist in applying a multigrid-like recursion scheme on a surrogate coarse-level function, typically obtained by adding a linear first order correction term. Global convergence results hold as long as the algorithm is based on a globally convergent method, independently of the recursion step structure. Here we are interested in studying the applicability of direct search algorithms in a multilevel optimization paradigm.

As a means to illustrate the issues addressed in our work, we devise an algorithm where a simple coordinate search method is employed as the underlying optimization algorithm. Multilevel recursion is implemented by a V-Cycle scheme, with and without Full Multigrid initialization.

First, we argue that the obtained algorithm enjoys error smoothing properties similar to those observed on traditional multigrid schemes for linear systems. Second, classical global convergence results for direct search algorithms guarantee that the same property holds for our method. Finally, we observe that the use of a multilevel strategy provides a significant gain in speed with respect to the underlying optimization algorithm, whose rate of convergence is usually very slow. As a result, traditional limitations on the problem size, typically to at most a few hundred variables, are overcome by the presented method. Furthermore, an attempt is made to make multilevel frameworks more suitable to a derivative-free context, by constructing approximate surrogate models which do not rely on gradient information. We support our arguments by reporting detailed numerical results on several test examples.

(Joint work with Alessandra Papini, Università degli Studi di Firenze)

A new approach for developing discrete adjoint models

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Adjoint techniques provide powerful tools for computational scientists, with important applications across the whole of science and industry. However, these techniques are not widely used, mainly due to the difficulty of implementing adjoint models. The main tool used in the development of adjoint models has heretofore been algorithmic differentiation (AD) tools, which are based upon the abstraction that a model is a sequence of elemental instructions. In this talk a new abstraction is investigated: that a model is a sequence of linear solves. Following this viewpoint, we describe the implementation of an open-source library (libadjoint) designed to assist in developing discrete adjoint models. The library implements the core algorithms for implementing such models, including assembly of the adjoint equations, managing the storage of forward and adjoint variables, and checkpointing algorithms to balance storage and recomputation costs. The library is applicable to any discretisation or equation, and is explicitly designed to be bolted-on to an existing forward model. We demonstrate the utility of the approach by adjoining models which are very difficult to differentiate with the AD approach.

Optimal flow control based on POD and MPC for the cancelation of Tollmien-Schlichting waves by plasma actuators

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The occurrence of a transition in the boundary layer above a flat plate is characterized by the formation of growing disturbances inside the boundary layer, which form two-dimensional waves called Tollmien-Schlichting waves. Successful damping of these waves can delay transition for a significant distance downstream, lowering the skin friction drag of the body.

We consider plasma actuators for active flow control. These actuators induce a body force which leads to a fluid acceleration, so the velocity profile is changed next to the surface. By optimal control of the plasma actuator parameters it is possible to reduce or even cancel the Tollmien-Schlichting waves and delay the turbulence transition.

We present a Model Predictive Control (MPC) approach for the cancellation of Tollmien-Schlichting waves in the boundary layer of a flat plate. The model that predicts the next flow field in a time horizon, has to fulfill the Navier-Stokes equations. Instead of solving a high-dimensional system, a low-order model description is used to perform the optimization. The reduced-order model is obtained with a Galerkin projection and an appropriate basis. We use Proper Orthogonal Decomposition (POD) in which the basis function are generated from numerical solutions or from experimental measurements. The optimization of the control parameters is performed within the reduced system.

Furthermore, we will show methods for improving the reduced model whose quality is verified in comparison to the results of a Finite Element based simulation for the considered problem.

Finally, we present our cancellation results with this MPC approach in a numerical simulation.

Uniqueness of an optimal solution in combinatorial optimization

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In this talk we show that tolerances of an optimal solution to a combinatorial optimization problem provide polynomially checkable necessary and sufficient conditions of uniqueness (non-uniqueness) of the optimal solution under consideration.

(Joint work with Alexey Goncharov and Andrey Prokofyev)

Matrix-free interior point method for large-scale optimization problems

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A redesign of Interior Point Methods (IPMs) for LP/QP problems will be addressed. It has two objectives:

(a) to avoid an explicit access to the problem data and to allow only matrix-vector products to be executed with the Hessian and Jacobian and its transpose; and

(b) to allow the method work in a limited-memory regime.

The new approach relies on the use of iterative methods with a specially designed preconditioner to solve the reduced Newton systems arising in optimization with IPMs. Numerical properties of the preconditioner will be analysed and its use will be illustrated by computational results obtained for very large scale optimization problems. The ability to work in a limited-memory regime makes the approach particularly attractive when solving problems which are so large that nothing but storing them is already problematic.

If time permits, numerical results of applying the approach to three classes of challenging problems will be presented: (a) relaxations of quadratic assignment problems, (b) quantum information problems, (c) sparse approximation problems arising in compressed sensing. These results will demonstrate that the matrix-free IPM approach involves very little computational cost which grows linearly with the problem dimension. Still the method retains the usual excellent IPMs convergence properties and solves difficult problems in the number of iterations that depends very little (if at all) on the problem dimension.

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New weak constraint qualifications with applications

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We present new constraint qualifications that are weaker than the usual Mangasarian-Fromovitz and Constant Rank Constraint Qualifications. In particular we solved the problem of finding which subset of the constraints must keep constant rank in order to obtain a constraint qualification. All of our conditions can be used to analyse global convergence of algorithms such as Sequential Quadratic Programming, augmented Lagrangians, interior point algorithms, and inexact restoration.

(Joint work with R.Andreani, P.J.S.Silva and M.L.Schuverdt.)

A semi-fixed Branch and Bound method for the traveling salesman problem

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In this paper, we present a heuristic algorithm based on the Branch and Bound (BB) method for the Traveling Salesman Problem (TSP), that is one of the combinatorial optimization problems. We call the proposed method the Semi-Fixed Branch and Bound (SFBB) method. The BB method is a method to find the optimal solution by searching the whole solution space, and consists of branching and bounding. The SFBB method is composed of three phases. In the first phase, it solves the plural approximate solutions in parallel by executing metaheuristics algorithms such as Tabu Search (TS), Ant Colony Optimization (ACO), and so on. After obtaining dozens of the approximate solutions from each algorithm, go to the next phase. In the second phase, it checks the solutions obtained in the first phase, and fixes several edges. It divides into a set of candidate edges (Ec) and a set of bounding edges (Eb). Ec is a set of edges emerging in many solutions. Eb is a set of edges rarely emerging in solutions. In the third phase, it executes the BB method in parallel for the subproblem with edges fixed by Ec and Eb. We perform computational experiments using the TSPLIB to evaluate the performance of the SFBB method. In the experiments, we use the PC cluster in our laboratory. In the parallel algorithm, we adopt Message Passing Interface (MPI) and Pthreads. It communicates between PCs with MPI, and assigns one thread to each core with Pthreads.

(Joint work with H.Ebara.)

A bilevel optimization approach to air flow control problem in the mine ventilation network

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The air flow control problem is a significant problem in the mine ventilation network and it has wide and important applications. In this talk, we investigate this problem and propose a bilevel optimization model to solve it. This bilevel model contains the upper-level problem which controls the air flow in the given region and the lower-level problem which describes the air flow equilibrium model and some control variables. Based on the derivative information of the flow equilibrium model in the lower-level problem, we implement the projected Barzilai-Borwein method to solve this bilevel model. Some preliminary numerical tests show the efficiency of our approach. The future works of the air flow control problem are also discussed.

Dynamic pricing and channel preference in a dual channel environment

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We investigate a retailer of a single product that employs two primary sales channels: 1) a physical channel (the "store") and 2) an online one. The retailer has the ability to influence the demand of each channel by using a different product price for each channel. Both channels' demands are satisfied using inventory that is held at the physical channel location. However, there is the following difference in the way demand is serviced. In each period (e.g. one day), the online channel demand is serviced at the end of the period using inventory that remains available after the physical store demand has been serviced during the period. Excess demands are backlogged and are not distinguished.

We obtain the structure of the retailer's dynamic pricing policy that maximizes the total discounted expected profit over a finite time horizon. Further, it is shown that the one period delivery flexibility of the online channel permits better demand uncertainty management and thus, the retailer may prefer selling through their online channel even if that channel's marginal profit is smaller than the marginal profit of selling through a more traditional channel.

(Joint work with Wen Chen, McCombs School of Business, The University of Texas, Austin, TX 78715 and Adam Fleischhacker Lerner College of Business and Economics, University of Delaware, Newark, DE 19716)

Pseudo-Boolean approach to market graphs analysis by means of the p-median model

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Recently Pardalos and his co-authors have applied cliques and maximum independent set models to the stock market analysis. In this paper we introduce a similar analysis by means of star graphs (induced by a feasible solution to the p-median problem) and compare its results on benchmark instances representing markets of Russia, Sweden and USA. Our algorithm for solving the p-median problem is based on the best known mixed Boolean linear programming formulation with the smallest number of non-zero coefficients in the objective function and corresponding linear constraints.

(Joint work with Mikhail Batsyn, Boris Goldengorin, Panos M. Pardalos, Pavel Sukhov.)

New class of optimization algorithms for multiple strip packing

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In a classical Strip packing problem we are given a list of rectangles (as input), and the objective is to find orthogonal packing of rectangles inside a unit width strip without rotations and intersections so that the height of packing is minimal. Because the problem is NP-hard, development of approximation algorithms is the main focus of research.

We consider some generalization of strip packing problem, so-called Multiple Strip Packing problem (MSP) where there are M strips of unit width instead of one. Initially MSP was addressed by Zhuk (2006) and then by other researchers. We consider new class of on-line optimization algorithms for MSP and analyze it analytically and experimentally.

Our results show that this class of algorithms outperform known algorithms for this problem. In particular, our average case analysis of this class of algorithms uses standard probabilistic model where for each rectangle its height and width are independent random variables uniformly distributed in [0,1]. We show that uncovered area of strips (total waste) for packing produced by our algorithms is substantially smaller than the waste of packings produced by the shelf algorithm proposed by Coffman and Shor in 1993.

Automatic evaluation and bounding of cross-derivatives: Optimal weights for high dimensional integration

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We present new methods for accurate evaluation and bounding of mixed derivatives of functions $f : \mathbb{R}^d \to \mathbb{R}$ by means of algorithmic differentiation. We assume that f is evaluated by a procedure that can be interpreted as a sequence of elementary arithmetic operations and intrinsic functions, which is the case in many practical applications. The new AD techniques aloud us to compute optimal weights required for construction of lattice rules. The latter is one of main techniques of Quasi-Monte Carlo for high dimensional integration. The weights define the embedding of f on a weighted (unanchored) Sobolev space. If the function at hand exhibits low effective dimension in truncation or superposition sense, accurate evaluation of certain mixed derivatives can be used to fix the weights. Otherwise, for the full dimensional case, we can efficiently compute using a new AD technique (product and order dependent) bounds for the mixed derivatives, resulting with an explicit expression for the recently introduced optimal "product and order" dependent weights. We show numerical results for examples related to finance.

Alternating direction method of multiplier: Theory and applications

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Alternating direction method of multiplier(ADMM) applies alternating technique on the KKT system of augmented Lagrangian function, which is a powerful algorithm for optimization problems with linear equality constraints and certain separable structures. In some applications, ADMM has excellent performance if we introducing some split techniques. In this talk, we show some techniques to make a good split and also demonstrate some preliminary result on the converegence of ADMM in general cases.

A new approach to compressed sensing thresholds

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Recent work in compressed sensing and related areas has shown that a sparse or simple solution to a large underdetermined system of equations can be recovered efficiently with very high or very low probability, depending on whether the parameters of the problem lie below or above a certain threshold. We present an approach for obtaining sparse recovery thresholds based on the probabilistic analysis of condition numbers for the conic feasibility problem. This approach also leads naturally to an analysis of sparse recovery problems with noise. The probability distribution of condition measures in optimization is well studied, and an overview of this work is given.

Limited-memory BFGS with diagonal updates

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We investigate a formula to solve limited-memory BFGS quasi-Newton Hessian systems with full-rank diagonal updates. Under some mild conditions, the system can be solved via a recursion that uses only vector inner products. This approach has broad applications in trust region and barrier methods in large-scale optimization.

Improved Branch-and-Bound algorithm for the maximum clique problem

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In this talk we suggest an exact algorithm for the Maximum Clique Problem (MCP). It is based on one of the fastest exact algorithms – MCS algorithm by Tomita, Sutani, Higashi, Takahashi and Wakatsuki (2010). The main improvement is the new initial ordering of vertices. We suggest a new order in which vertices are colored on each step; this new order reduces the overall number of search tree nodes for different instances of MCP. Our ordering is based on one of the best heuristic algorithms – Fast Local Search for the Maximum Independent Set Problem by Andrade, Resende and Werneck (2008). We run this algorithm to find several cliquesand then order vertices so that vertices from the larger found cliques are assigned a color. As a result, large search sub-trees related to such vertices are pruned earlier due to the small number of colors assigned to these vertices. We also suggest a new fast coloring algorithm which gives a better upper bound for the maximum clique. Computational results showing a comparison with the original MCS algorithm are presented.

(Joint work with Mikhail Batsyn, Boris Goldengorin, Panos M. Pardalos.)

Optimal paths in graphs, powers with an idempotent operation, and an application to analysis of agglomerations

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A dynamic model with a finite set of states without and with discounting is considered here from perspectives of dynamic programming and idempotent (tropic) mathematics. The scheme of dynamic programming was studied by many authors, however, some natural and principally important conclusions have been missed. Firstly, under natural conditions, similarly to the initial part of the optimal path with sufficiently large horizon, the final part of the path can be constructed backwards (in the inverse time) stepwise by use of a function which is referred here as the second value function. This function corresponds the left eigenvector of the matrix of utilities in an algebra with an idempotent operation, while the first value function corresponds the right eigenvector. Secondly, the T-step optimal path under a sufficiently large horizon T has a three-part structure. A representation of the T-th power of the matrix of utilities with the idempotent operation corresponds this three-part structure. The three-part structure of optimal paths and its relation to the behavior of powers of matrices in the idempotent algebra are studied. As an application of the results we study some questions of modeling agglomerations in spatial economics. A peculiarity of a spatial system is a presence of two sets of agents: stationary agents which are linked to other agents posed in the same area and free agents which are able to move their activity (links) to another area.

Methods of combinatorial optimization as applied to protein structures

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The present work is a continuation of the research program which aims to model protein and other biopolymer structures through methods of Mathematical Programming. It is found that an elementary knowledge of Combinatorial Optimization techniques is enough to obtain a reasonable agreement with data of the scientific literature. The data corresponding to Amide Planes have been obtained by intensive statistical analysis of peptides. We present here a unified approach based on perturbations of bond and dihedral angles which is able to derive the alpha-helix structure as a byproduct. The fundamental assumption is the consideration of continuous and differentiable curves through special sets of atom sites and the existence of evenly spaced consecutive atom sites according the Euclidean distance. Right circular helices are the only 3-dimensional curves such that the consecutive atom sites are also evenly spaced along them, which results from the theorem on homogeneous functions. The observed connection of each atom site of a biopolymer to no more than four nearest neighbours is also derived, by introducing the Ansatz for the coordinates with the property of evenly spaced euclidean distances and the desirable assumption of local equilibrium on the neighbourhood of each atom site of the protein backbone. An application to the perturbation of Ramachandran plots and and the analysis of robustness of the protein structures is also presented. Some works of the author which contain a detailed treatment can be found at the journals Genetics and Molecular Biology, Global Optimization and at Encyclopedia of Optimization - 2nd edition (eds. C. Floudas , P. Pardalos) and at chapters of the indexed BIOMAT series of books (ISI - Web of Science, Scientific Proceedings Citation Index).

Facilitating green building adoption - an optimization based decision support tool

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The US Environmental Protection Agency defines green buildings as the practice of creating structures and using processes that are environmentally responsible and resource-efficient throughout a building's life-cycle from site selection to design, construction, operation, maintenance, renovation and deconstruction.

The adoption of green building norms in India is a relatively new phenomenon. The Indian Green Building Council (IGBC) has been the torch bearer for this effort since 2001. There are three major green building guidelines currently being adopted in India: (1) LEED-New Construction (LEED-NC); (2) GRIHA by The Energy and Resources Institute (TERI) that was established voluntarily to rate buildings; and (3) LEED-INDIA released by the Indian Green Building Council which is inspired by LEED-NC and includes alterations based on Indian construction environment.

The decision to opt for green construction and the level of green aspirations is constrained by the extra cost of going green, i.e. the green premium. The level of environment friendliness, given by the rating of the building, is not arrived at in a scientific manner by considering the options and their cost implications. Risk averse owners, in spite of their desire to go green, are hindered by a lack of information on the various options and ability to decide which options to choose. This information if made available as a decision support tool can be valuable in bringing green buildings into the mainstream. The non availability of such a tool is a major barrier in the growth of the green building movement (USEPA report on *Removing market barriers to green development*).

The objective of this work is to develop an optimization based decision support tool that can be used to either arrive at the optimal green rating given the budget and choice constraints; or at the optimal green premium given the green rating aspirations. These can help a builder optimize green ratings or greening costs, as desired, or by a policy maker to come up with appropriate and effective policies. The Indian GRIHA rating guidelines are used as inputs for measuring the green rating of a building. In addition sensitivity to costs, of socially important parameters such as use of solar energy, fly-ash etc., of choices made for achieving desired green ratings are studied. This can help drive appropriate policy initiatives for adoption of such technologies.

(Joint work with D. Roychowdhury and P.D. Jose.)

Hessian-based topology optimization in fluid mechanics

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This paper presents an Hessian-based approach for the topology optimization of viscous ducted flows. Since in shape optimization the number of design variables is relatively small, especially when shape parameterization is used, the cost of computing the exact Hessian matrix, which scales with the number of design variables, is affordable. In contrast, in topology optimization, the optimal nodal porosity distribution is sought in order to minimize the objective at hand and, thus, the number of design variables becomes prohibitively large for the computation of the exact Hessian, especially for 3D cases. So far, topology optimization has extensively been used for structural optimization and only a few different applications can be found in the literature. Among them, the topology optimization of flows, using exclusively gradient based approaches. Since the computation of the exact Hessian matrix for topology optimization problems is too expensive, the truncated Newton approach to accelerate the convergence of the optimization loop is proposed; here, the Newton equations are solved iteratively using the conjugate gradient algorithm, until partial convergence, without computing the exact Hessian matrix values. Instead, Hessian-vector products are computed at each cycle with a cost independent of the number of design variables. These are efficiently calculated using a combination of the adjoint method and direct differentiation. Usually a small number of conjugate gradient iterations is required for the truncated Newton algorithm to outperform conventional descent algorithms. In order to accelerate convergence even more, the hybridization of first order gradient methods with the truncated Newton approach is investigated.

The proposed topology optimization algorithm is applied to the optimal design of ducted flows by minimizing the total pressure losses between the inlet and the outlet of the duct.

Simplicial Lipschitz optimization without the Lipschitz constant

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Lipschitz optimization is one of the most deeply investigated subjects of global optimization. The main disadvantage of Lipschitz methods is the requirement to provide the Lipschitz constant of the objective function. In this talk we develop a simplicial version of Lipschitz optimization without the Lipschitz constant. The efficiency of the proposed algorithm is evaluated experimentally and compared with the results of other algorithms.

The duration problem with multiple exchanges

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The multiple-choice duration problem has, as objective, maximizing the time of possession of relatively best objects. we show that for the m-choice problem there exist m critical times such that, when there are k choices still to be made, the optimal strategy selects a relatively best object if it appears at or after the k-th critical time.

Adjoint-based nonlinear optimization of complex systems governed by partial differential equations using high-performance computing techniques: Implementation issues and examples

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The simulation of complex systems governed by partial differential equations often presents several challenges: the phenomenon modeling, domain discretization, solving linear systems, visualization, among others. Solving linear systems is particularly difficult when large scale problems are involved because the time of resolution of a system may be too large, making its analysis difficult (or impossible in many cases). Supercomputers are used to solve the above mentioned task, comprising thousands of computers connected so as to function as a single large entity, with the aim to increase the processing capacity and storage available to users. Such large amount of computational power allows to solve major problems associated with fluid and solid mechanics, biology, geophysics, among other areas of science.

With the simulator already implemented and capable of using efficiently the resources of a supercomputer, a question remains to be answered: If the system depends on parameters, what would the optimal parameters be to minimize a given objective function?

In this work we present a high fidelity adjoint based optimization method using high-performance computing techniques, capable of efficiently running in thousands of cores.

We will show an implementation of the discrete adjoint method to compute derivatives of a given objective function. With those derivatives, gradient-based optimization methods are used to achieve local optima for the system's parameters. The implementation is integrated into a computational mechanics code called Alya, which is capable of solving different multi-physics problems, in a coupled way, and is designed for running in large scale supercomputing facilities with linear scalability. The integration keeps the original scalability and efficiency, and introduce minimal code modifications.

Finally, speedup results of test problems will be shown, using different meshes, from hundreds to millions of elements, and several processes running in a distributed memory supercomputer.

Optimal Boundary Control for Nonlinear Hyperbolic Conservation Laws with Source Terms

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Hyperbolic conservation laws arise in many different applications such as traffic modelling or fluid mechanics. The difficulty in the optimal control of hyperbolic conservation laws stems from the occurrence of moving discontinuities (shocks) in the entropy solution. This leads to the fact that the control-to-state mapping is not differentiable in the usual sense.

In this talk we consider the optimal control of a scalar balance law on a bounded spatial domain with controls in source term, initial data and the boundary condition. We show that the state depends shift-differentiable on the control by extending previous results for the control of Cauchy problems. Furthermore we present an adjoint-based gradient representation for cost functionals. The adjoint equation is a linear transport equation with discontinuous coefficients on a bounded domain which requires a proper extension of the notion of a reversible solution. The presented results form the basis for the consideration of optimal control problems for switched networks of nonlinear conservation laws.

DC Programming Approaches for Discrete Portfolio Optimization under Concave Transaction Costs

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The goal of this paper is to present an efficient method for solving discrete portfolio optimization under concave transaction costs. By using a suitable penalty parameter, we can reformulate this nonseparable, nonconvex, nonlinear integer program as a DC program which could be solved by DCA. We also compare its solution to that offered by a global method as Branch and Bound where DC relaxation is used for lower bounding. Some preliminary computational results are reported.

A deterministic algorithm for multi-objective optimization problems

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Optimization problems involving multiple, conflicting objectives are often approached by aggregating the objectives into a scalar function and solving the resulting single-objective optimization problem. In contrast, in this paper, we are concerned with finding a set of optimal trade-offs, the so-called Pareto-optimal set. Many numerical methods for constructing Pareto-set approximations have been proposed so far. Most of them are heuristic, i.e. they don't guarantee the optimality of the found solutions. We formally define notions of Pareto and epsilon-Pareto sets and prove some important properties of these sets. We also propose a deterministic algorithm to construct finite epsilon-Pareto approximations. The algorithm is based on non-uniform space covering techniques. Its convergence in a final number of steps is formally proved. The serial and parallel implementations of the proposed approach are also discussed. We experimentally compare the proposed algorithm with some other well-known approaches to constructing Pareto-front approximations. Experiments have shown that the proposed deterministic algorithm is highly competitive with the state-of-the-art multiobjective optimization methods.

Numerical procedures for optima control problems described by higher index differential-algebraic equations

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The paper presents a new numerical procedure for optimal control problems described by higher index differential-algebraic equations. The procedure does not require differentiation with respect to time of some algebraic equations in order to reduce the index of DAEs. Instead it is based on an integration procedure which copes efficiently with higher index differential-algebraic equations . The procedure is also based on reduced gradients of all functional defining the optimal control problem. They are evaluated with the help of properly defined adjoint equations whose discretization is consistent with the discretization of system equations. The consistent initialization is done by applying the Pantelides procedure. Numerical examples are provided to show efficiency of the proposed procedure.

Solving regularized convex problems in huge dimensions via greedy, randomized, serial and parallel coordinate descent

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We develop a randomized block-coordinate descent method for minimizing the sum of a smooth and a simple nonsmooth block-separable convex function and prove that it obtains an eps-accurate solution with probability at least $1-p$ in at most $O[(2n/eps)log(1/p)]$ iterations, where n is the dimension of the problem. For strongly convex functions the method converges linearly. This extends recent results of Nesterov [Efficiency of coordinate descent methods on huge-scale optimization problems, CORE Discussion Paper #2010/2], which cover the smooth case, to composite minimization, while at the same time improving the complexity by the factor of 4 and removing eps from the logarithm. More importantly, in contrast with the aforementioned work in which the authors achieve the results by applying their method to a regularized version of the objective function with an unknown scaling factor, we show that this is not necessary, thus achieving true iteration complexity bounds. In the smooth case we also allow for arbitrary probability vectors and non-Euclidean norms. We will also mention new iteration complexity results for a greedy and a randomized parallel variant of coordinate descent. In the second part of the talk we demonstrate numerically that the algorithm is able to solve huge-scale $L1$-regularized support vector machine and least squares problems with billion variables. Finally, we present computational results with a GPU-accelerated parallel version of the method, on truss topology design and other problems, achieving speedups of up to two orders of magnitude when compared to a single-core implementation in C.

Piecewise monotonic regression algorithm for problems comprising seasonal and monotonic trends

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We consider piecewise monotonic models for problems comprising seasonal cycles and monotonic trends. In contrast to the conventional piecewise monotonic regression algorithms, our algorithm can efficiently exploit a priory information about temporal patterns.

Our approach is based on establishing monotonic relations between the observations that compose the data set. These relations make the data set partially ordered, and allows us to reduce the original data fitting problem to a monotonic regression problem under the established partial order. The latter is a large-scale convex quadratic programming problem. It is efficiently solved by the recently developed Generalized Pool-Adjacent-Violators (GPAV) algorithm.

Newton's method for equations with geometric constraints

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A Newton-type method for set-valued maps, recently developed by Dias and Smirnov (Nonlinear Analysis, Vol. 75, 2012, pp. 1219-1230), is a general tool suitable to solve in a unified manner inclusions, systems of inequalities, and systems of nonlinear equations with geometric constraints. Under natural conditions this method quadratically converges for general inclusions and solves in a finite number of iterations generic systems of linear inequalities. In this talk we discuss complexity issues related to this method. The emphasis is given to the estimates for the number of iterations needed to reach the region of quadratic convergence. The results are illustrated by examples from control theory. We apply the set-valued version of Newton's method to systems of nonlinear equations with geometric constraints generated by control systems and show how this approach allows to solve the nonlinear problem of compensation of J2 perturbations for formation flying of two satellites. It is supposed that the chief satellite moves passively along a circular orbit and the deputy satellite is equipped with a thruster oriented along the geomagnetic field or along an axis fixed in the inertial space.

Convex duality for growth optimal portfolio insurance

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The Growth Optimal Portfolios (GOP), which maximize log-power utility, have many attractive features and play an important role in modern theoretical finance. From a practical prospective they suffer from a high riskiness. We propose a simple method of downside protection of the GOP. At first, by solving convex duality problem we find payoff of the GOP at the terminal date. Then we introduce inequality constraint that portfolio value at terminal date must stay above some floor, which leads to kink formation in optimization problem. However we still show that problem can be solved within convex duality framework and optimal payoff of the protected GOP can be represented as call option on non-protected portfolio. Finally, by using standard Black-Scholes model we derive closed form solution for optimal dynamic investment proportion. We provide illustrations of proposed algorithm and suggestions on improvement of its performance.

A new model for Moon's origin and its modeling via nonlinear optimization

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The origin of the Moon has been investigated for long time, most theories presented in the past are now rejected due to differences in the rocks of Moon and Earth. We propose a four-body model where Moon is a satellite taken by Earth from a large body passing close at about 9500 BC, when Ice Age ended suddenly with the associated Atlantis civilization. We show that this theory explains details in myths, especially those of Arcadia, and religions, claiming also that Aphrodites is Moon and not Venus, as De Grazia first proposed. We show how the capture can be formulated as a nonlinear optimization problem.

Structure in optimization

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The purpose of this talk is to explore problem structure of in optimization. We will assume that the function naturally decomposes into known functions. Some of the best known examples of such functions are separable functions or additively decomposed functions, partially separable functions (advocated by Griewank and Toint) and group partially separable functions (advocated by Conn, Gould and Toint). The last class of functions forms the input to LANCELOT. We will show how these structures lead to development of methods and parallelization. In these examples the functions are additively decomposed.

Coleman and Verma introduced structure in optimization as a sequential computation of blocks of variables. To illustrate structured computation we follow Coleman and Verma. Assume that the objective function f is on the form f(x) = g(x,y) where g is a function of n+m variables x and y where y satisfies a linear system of equation A(x) y = F(x) for some nonlinear function F. Here A is a nonsingular m x m matrix that depends on x. For a given value of x the computation of z=f(x) will be: Solve for y: A(x)y = F(x); Update z: z= g(x,y); This can be generalized and Coleman and Verma argue that objective function are naturally expressed in a high level structured form.

Factorable functions and factorable programming problems were developed from 1967 through 1990 and is an early example of structure in nonlinear optimization. We will explore the relationship between algorithmic differentiation (AD) and the definition of factorable functions. However, the main use of factorable programming is in the structure of the derivatives and global optimization.

The gradient is a sum of monads (vectors) and the Hessian matrix is a sum of dyads or a sum of outer products. We show that using source transformation of a simple Fortran 90 implementation of a classical example due to Jackson and McCormick from 1986 gives the desired structure.

Experimental analysis of heuristics for the single machine scheduling problem $\mathbf{1}|pmtn; p_j = p|SUMw_jC_j$

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The preemptive single machine scheduling problem of minimizing the total weighted completion time with equal processing times and arbitrary release dates is one of the three single machine scheduling problems with an open computational complexity status. In this talk we discuss our computational study of the problem $1|pmtn; p_j = p|SUMw_jC_j$ solved by means of different heuristics. The WSRPT (weighted shortest remaining processing time) rule is not optimal but returns an optimal solution within reasonable CPU time for almost all involved instances.

(Joint work with Daniel Berend, Boris Goldengorin, Panos M. Pardalos.)

Penalty decomposition methods for probabilistically constrained convex programs

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We consider in this paper probabilistically constrained convex program (PCCP) in finite discrete distribution case. The problem can be reformulated as a mixed-integer convex program (MICP) which is in general NP-hard. By exploiting the special structure of the probabilistic constraint with discrete distribution, we present a penalty decomposition for finding a suboptimal solution of PCCP. This method is based on applying alternating direction method to a penalty decomposition formulation of the MICP reformulation, in which a convex programming subproblem and a 0-1 knapsack subproblem are solved alternatively at each iteration of the algorithm. We show that the 0-1 knapsack subproblem has closed form solution in the case of equal probabilities. Convergence properties of the method are established under mild conditions. We report preliminary computational results which show that the proposed penalty decomposition method is promising for finding good quality suboptimal solutions and compares favorably with other existing approximation methods for large-scale PCCPs.

(Joint work with Xiaodi Bai, Xiaojin Zheng and Jie Sun.)

A variation of the pure adaptive random search

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A variation of the pure adaptive random search is considered. The key concept of the presented algorithm is a perspective region - a region that is likely to contain the sought-for extremum of the function being optimized. A distribution of solutions is a mixture of uniform distributions inside and outside the perspective region. Parameters of the algorithm are investigated according to their meaning for the optimization process. The algorithm has shown its effectiveness on different test functions characterized by their complexity for optimization.

GPU accelerated greedy algorithms for compressed sensing

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Greedy algorithms have proven to be an efficient means of solving the combinatorial optimization problem associated with compressed sensing. In this talk we describe an implementation for graphical processing units (GPUs) of hard thresholding, nomalized iterative hard thresholding, hard thresholding pursuit, and a two stage thresholding algorithm based on the algorithms compressive sampling matching pursuit and subspace pursuit. The GPU acceleration of the matrix vector products in these algorithms results in support set identification (order statistics calculations) being a significant portion of the computational burden; the software includes adaptive approximate order statistics algorithms to remove alleviate the computational cost of the support set identification. The software permits large-scale testing at dimensions currently unavailable in the literature. The GPU implementations exhibit fifty to one hundred times acceleration over serial implementation on standard server grade CPUs.

(Joint work with Jeffrey D. Blanchard, Grinnell College.)

Network based computing environment for solving optimal control problems

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The aim of the presentation is to show the current state of work on computing environment (Interactive Dynamic Optimization Server) which enables solving optimal control problems by using Internet services. The environment aims at solving control problems described by ordinary differential equations, differential-algebraic equations (also with higher index) and partial differential equations. Currently solvers which are available within IDOS are: several solvers which are based on the discretization of differential equations and optimization solvers suitable for solving large scale problems such as Ipopt and Knitro; solvers based on adjoint equations of systems equations (ordinary differential equations, higher index differential-algebraic equations, partial differential equations); solvers applying multiple shooting method. The computing environment is equipped with dynamic optimization modeling language â DOML which is an extension of Modelica language. The presentation will focus on the scope of optimization solvers included in the environment; elements of DOML language; mechanism of adding new solvers to the environment. Also the use of the environment IDOS will be discussed.

(Joint work with J. Blaszczyk, R. Pytlak.)

Loan portfolio reservation in condition of incomplete information

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A change of shares of credits portfolio is described by Markov chain with discrete time. A credit state is determined on as an accessory to this or that group of credits depending on presence of indebtedness and its terms. We use a model with discrete time and fix the system state through identical time intervals - once a month. We consider a stable economic situation when the transition probabilities are supposed to be constant.

It is obvious that the matrix of transitive probabilities is incompletely known and its values are specified constantly according to the analysis of a portfolio. We considered three methods approaches to matrix estimation and two ways to forecast the share of problem loans taking into account the uncertainty of the transition probabilities matrix. There are a confidence estimation method and a simulation method. Criterion of a choice is an accuracy of the forecast of a share of problematic loans and necessary reserves.

We consider the estimation problem of a share of problematic loans and propose a method to calculate necessary reserves on this base. A value of necessary reserves depends on quality and structure of the portfolio. On the one hand reserves should provide a low probability of the default; on the other hand they impact on a profitability of the portfolio. We consider two ways of describing a credit portfolio dynamics: a regular Markov chain in which we do not take into account repaid loans and renovation of the portfolio and a scheme which included quotation a new loan quotation and quotation a repaid loan quotation as possible states of a loan.

In the first way we investigate a steady-state behavior of the loan portfolio shares, in the second way we study the profitability of loans from delivery to its repayment. Methods to calculate necessary reserves are studied for both schemes.

Optimization and stabilization of traffic flow on the base of the hybrid model

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Hybrid models are widely used for traffic flows modeling. The original mathematical model of vehicles movement in the form of a dynamic hybrid system is suggested. The model describes the motion of vehicles on lanes by differential equations based on the modification of the Intelligent Driver Model (IDM). The change of a lane is a piece-wise constant discrete component. Some simplifications have been brought in equation IDM. Numerical parameters of the equations of acceleration and deceleration are chosen taking into account statistical data on car movement in Russian cities. Sufficient conditions of a stationary solution existence for the hybrid system are obtained, the stabilization problem is studied.

We consider a multicriteria problem of the effective choice the optimal operating mode of a traffic light are studied on the base of the suggested hybrid model and its computer simulation.

A Fortran software package for piecewise monotonic data smoothing combined with a test for trends

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A Fortran software package has been developed for providing a solution to the following data smoothing problem. Suppose n measurements of a smooth function include substantial random errors, so that the number of peaks and troughs of the data may be unacceptably larger than the number of turning points of the function. Demetriou & Powell (1991) proposed making the least sum of squares change to the data subject to a limit, q say, on the number of sign changes of their first divided differences, but usually a suitable value of q is not known in advance. It is shown how to obtain automatically an adequate value for q by employing Powellâ test that attempts to distinguish between trends and data errors. Specifically, if there are trends, then the monotonic sections of a tentative approximation are increased by one, otherwise this approximation seems to meet the trends and the calculation terminates. The numerical work required per iteration, beyond the second one, is quadratic in n. The software package has been tested on a variety of data sets showing a performance that provides in practice shorter computation times than the complexity in theory. Driver programs and numerical examples with output are provided to help new users of the method.

(Joint work with I. C. Demetriou.)

Higher-order discontinuous Galerkin methods for temporal discretization of parabolic optimal control problems

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In this talk we discuss an efficient realization of higher-order discontinuous Galerkin methods for optimal control problems governed by parabolic differential equations. Moreover we present a priori error estimates for a post-processing approach based on superconvergence at Radau points.

A composite SQP-Newton method for nonlinear programs

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We consider a sequential quadratic programming type algorithm with local quadratic convergence for nonconvex nonlinear programs. While SQP-methods feature local quadratic convergence under favourable conditions, it is known that for nonlinear programs with degenerate constraints superlinear convergence gets lost for the standard method. In order to deal with this problem, we study the SQP-method from the point of view that the next iterate is a function value of the previous iterate. In some cases, this function can be shown to be piecewise differentiable. This leads to the idea of combining SQP and Newton methods. More specific, the algorithm we propose consists of a simplified quadratic subproblem, which alone would result in linear convergence at best, and an additional Newton step in order to achieve local superlinear convergence. Some preliminary numerical results are presented.

An augmented Lagrangian trust region algorithm for nonlinear programming

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In this paper, we present a new trust region method for equality constrained optimization. The method is based on the augmented Lagrangian function. Its main innovation lies in that we minimize an approximation to the augmented Lagrangian function in trust region in each subproblem. Novel strategies to update the penalty parameter and the Lagrangian multiplier are also proposed. Under very mild conditions, global convergence of the algorithm is proved. Preliminary numerical experience for problems with equalities from the CUTEr collection is also reported. It indicates that for problems with equality constraints the new method is as effective as and competitive with the famous algorithm LANCELOT. Also, we extend this method to general nonlinear programming problems.

Sparse optimization methods for seismic data regularization

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Due to the influence of variations in landform, geophysical data acquisition is usually sub-sampled. Therefore, proper data regularization and recovery is a necessary task. Reconstruction of the seismic wavefield from sub-sampled data is an ill-posed inverse problem. It usually requires some regularization techniques to tackle the ill-posedness and provide a stable approximation to the true solution. In this talk, we consider the wavefield reconstruction problem as a compressive sensing problem. We solve the problem by constructing different kinds of regularization models and study sparse optimization methods for solving the regularization model. The l_p-l_q model with $p = 2$ and $q = 0, 1$ is fully studied. The projected gradient descent method, alternating directions method and an l_1-norm constrained trust region method are developed to solve the compressive sensing problem. Numerical results demonstrate that the developed approaches are robust in solving the ill-posed compressive sensing problem and can greatly improve the quality of wavefield recovery.

Tolerance based BnB algorithm for the weighted maximum independent set problem

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In this paper we design a new heuristic tolerance-based algorithm for solving the Weighted Independent Set problem (the WIS, for short). Our algorithm is based on the polynomially solvable special case of WIS which is defined on trees (the WIST, for short). We show that an optimal solution and all its tolerances for the WIST might be simultaneously found by the adjusted Chen et al. dynamic programming algorithm in $O(n)$ time. Based on this procedure we offer a heuristic algorithm for the WIS, which runs in $O(m^2 \log(n)/n)$ time. We also present several computational experiments for its approximation ratio, they showed good enough results for some sparse graphs.

(Joint work with Boris Goldengorin, Dmitry Malyshev, Panos M. Pardalos.)

Movement of solids in multiphase viscous medium

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In the framework of the energy optimization of the flow of solids viscous medium [D.S.Zavalishchin, S.T.Zavalishchin. Dynamic optimization flow. Moscow: Nauka, FIZMATLIT, 2002] studied new classes of optimal control movement of solids in multiphase viscous medium.

The researches deal with a model of a cylindrical body displacements through border of two viscous media. The system of the differential equations describing a rigid body movement through the boundary of a viscous media is obtained. It allows to model various modes of such movement. This model enables one to set up the problem of displacements of a cylindrical body for optimum energy consumption, the time and distance of the displacement being given. The problem has a number of special features. First, it is irregular because the Euler-Lagrange equations do not contain controls in an explicit form, and, hence, the optimal controls cannot be determined in terms of the state and adjoint variables. Second, as it was found out, there are impulse components in the control forces and momentums optimum programs. Therefore, the classical variational techniques cannot be directly applied to find these programs. The third feature follows from the second one and consists of calculating the energy consumption. So, the speech goes about a new set of problems being topical from the viewpoint of the theory of singular or degenerate solutions of dynamic optimization problems. The totality of the problems solved can be used in both the applied theory of singular dynamic optimization problems and design of perspective samples of new machines.

On some variants of locally convergent affine-scaling methods for linear semidefinite programming problems

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In this paper we consider the standard linear programming problem. Some variants of primal and dual affine-scaling methods for finding its solution are proposed. Although the methods have many properties of interior point methods, their construction completely avoid using the idea of barrier functions. Actually, these methods are obtained as special techniques for solving the system of necessary and sufficient conditions for a pair of mutually dual linear semidefinite programming problems. We consider the feasible and unfeasible variants of methods. The methods can be treated also as generalizations of barrier-projection methods proposed earlier for solving the linear programming problems. Our main goal is to show that the local convergence with at linear rate takes place for these methods under some assumptions. The Ostrowsky theorem is used for proving this result. We also consider the primal and dual affine scaling Newton's methods are prove their local convergence with at superlinear rate.

On proximal gradient method for a class of nonsmooth convex minimization problems

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Consider a class of nonsmooth convex optimization problems where the objective function is the composition of a strongly convex differentiable function with a linear mapping, regularized by the sum of both l_1-norm and the group reproducing kernel norm of the optimization variables. This class of problems arise naturally from many applications in such as sparse group Lasso and other fields, which is a popular technique for variable selection. An effective approach to solve such problems is by proximal splitting method. In this paper we establish and study its iterative and subiterative algorithms for the class of the problems.

(Joint work with Shu Wang.)

Sparse optimization techniques for solving multilinear least-squares problems with application to design of filter networks

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The multilinear least-squares (MLLS) problem is an extension of the linear least-squares problem. The difference is that a multilinear operator used in place of a matrix-vector product. The MLLS is typically a large-scale problem characterized by a large number of local minimizers. Each of the local minimizers is singular and non-isolated. The MLLS problem originates, for instance, from the design of filter networks.

For the design of filter networks, we consider the problem of finding optimal sparsity of the sub-filters that compose the network. This results in a MLLS problem augmented by an additional constraint that poses an upper limit on the number of nonzero components in the solution. This sparse multilinear least-squares problem is NP-hard. We present an approach for approximately solving the problem. In our numerical experiments, a greedy-type sparse optimization algorithm is used for designing 2D and 3D filter networks.

The efficiency of our approach is illustrated by results of numerical experiments performed for some problems related to the design of filter networks.

(Joint work with Mats Andersson, Oleg Burdakov and Hans Knutsson.)

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