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40th Workshop

LARGE SCALE NONLINEAR OPTIMIZATION

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ABSTRACTS
of the invited lectures

Simple Methods for Extremely Large-Scale Convex Problems

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The need to solve extremely large-scale (10^4–10^6 variables) convex optimization problems, such as those arising in medical imaging, shape design of mechanical structures and more, enforces one to reconsider simple gradient-type algorithms as the only methods of choice, since more sophisticated algorithms (such as interior point) require in a single iteration a number of arithmetic operations that are prohibitively large. We propose in this talk a new subgradient-type method, the "Non-Euclidean Restricted Memory Level (NERML) method", for minimizing large-scale nonsmooth convex over "simple" domains. The characteristic features of NERML are: (a) The possibility to adjust the scheme to the geometry of the feasible set, thus allowing essentially dimension-independent rate of convergence, which are nearly optimal in the information complexity sense; (b) flexible handling of accumulated information, allowing for trade-off between the level of utilization of this information and the iterations' complexity.

We briefly mention extensions of NERML to finding saddle points and solving variational inequalities with monotone operators. Finally, we report on encouraging numerical results of experiments with test problems of dimensions in the order of 10^5–10^6.

A Unified View of Existence of Optimal Solutions, Duality, and Minimax Theory

Dimitri Bertsekas
MIT
USA

We explore some intimate connections between several fundamental issues in nonlinear programming and zero sum game theory. The main tool is a single, powerful new theorem on the nonemptiness of the intersection of a nested sequence of closed sets. Starting from this theorem, we give a unified analysis of the major conditions for preservation of closedness of sets under linear transformations, for preservation of lower semicontinuity of functions under partial minimization, for existence of optimal solutions in (nonconvex) constrained optimization, for the absence of a duality gap, and for min-max=max-min.

Fast linear algebra for multiarc trajectory optimization

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Le Chesnay, France

Interior-point algorithms applied to optimal control problems have very sparse Jacobian matrices, e.g. band matrices in the case of a single arc in the absence of constant time optimization parameters.

In the first part of the talk, we discuss how to design fast linear solvers adapted to this case, and their combination with the refinement of discretization. The second part deals with multiarc problems. We show how to solve quickly the Newton steps when the connction graph is a tree, and give indications on the general case.

An $O(n^2)$ algorithm for isotonic regression problems

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We consider the problem of minimizing the distance from a given n-dimensional vector to a set defined by some number of constraints of the form $x_i \leq x_j$. The structure of these constraints can be presented by an acyclic directed graph, which induces a partial order of the components x_i. This problem is known as the isotonic regression problem (IR). It has important applications in statistics, operations research and signal processing. They are often characterized by a very large value of n. For such large-scale problems, it is of great practical importance to develop algorithms whose complexity doesn't rise with n too rapidly. The existing optimization based algorithms and statistical IR algorithms have either too high computational complexity or too low accuracy of the approximation to the optimal solution they generate.

We introduce a new IR algorithm, which can be viewed as a generalization of the Pool-Adjacent-Violator (PAV) algorithm, from completely to partially ordered data. Our algorithm combines both low computational complexity $O(n^2)$ and high accuracy. This allows us to obtain sufficiently accurate solutions to the IR problems with thousands of observations.

Augmented Lagrangian Method for Large-Scale Linear Programming Problem

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We propose to use a new auxiliary function close to augmented Lagrangian for solving primal and dual LP simultaneously. Our approach has the following main advantage: after single unconstrained maximization of auxiliary function we obtain the exact 2-norm projection of a point onto the solution set of primal LP problem. The auxiliary function has a parameter (similar to the penalty coefficient) which must be more or equal some threshold value. This value is found under regularity condition. Using this result, we maximize once again the auxiliary function with changed Lagrangian multipliers and obtain the exact solution of dual LP problem. The exact primal and dual solutions of LP problems are obtained in a finite number of iterations with *arbitrary* positive value of the parameter. The auxiliary unconstrained maximization problems are solved by fast generalized Newton method.

The proposed approach was applied to primal linear programming problems with very large number ($\approx 10^6$) of nonnegative variables and moderate ($\approx 10^4$) number of equality type constraints. The results of computational experiments are given.

Exact penalty methods for generalized Nash problems

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A generalized Nash problem (GNP) is a Nash problem where the feasible set of each player depends on the other players' variables. This kind of problems can not be reduced to a variational inequality (VI) directly, as it is usually done for Nash problems, and very few solution algorithms have been proposed to date. We propose an exact penalty approach to the GNP whereby the GNP is reduced to a (unconstrained) nonsmooth Nash problem. An updating scheme for the penalty parameter is studied that, when used in conjunction with any algorithm for the solution of the nonsmooth penalized Nash problem, guarantees that a correct value of the penalty parameter is found in a finite number of steps. We also propose a smoothing method for the solution of the nonsmooth Nash problem derived from the application of the penalty technique.

This is a joint work with J.-S. Pang

Parallel Interior Point Solver for Very Large Scale Nonlinear Optimization

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Very large optimization problems with millions of constraints and decision variables display usually some special structure. The key to efficient solution of such problems is the ability to exploit the structure. We have developed a structure-exploiting parallel primal-dual interior-point solver for nonlinear programming problems. The solver can deal with a nested embedding of structures. Hence very complicated real-life optimization problems can be modeled.

Its design uses object-oriented programming techniques. Different matrix structures are implemented as subclasses of an abstract matrix class. This abstract matrix class contains a set of virtual functions (methods in the object-oriented terminology) that:

(i) provide all the necessary linear algebraic operations for an interior point method, and

(ii) allow self-referencing.

The program OOPS (Object-Oriented Parallel Solver:
http://www.maths.ed.ac.uk/ gondzio/parallel/solver.html) can efficiently handle very large nonlinear problems.

The efficiency of the solver is illustrated with problems known from the literature: applications arising from telecommunication and financial engineering. Numerical results are given for the solution of nonlinear financial planning problems. For small-to-medium scale problems (with sizes below 1 million variables) the solver is often an order of magnitude faster than Cplex 7.0. Large scale problems (with sizes over 50 million decision variables) are solved on parallel platforms: OOPS achieves an almost perfect scalability.

This is a joint work with Andreas Grothey.

Constraint preconditioners for large-scale nonlinear optimization

Nick Gould
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The solution of simple "model" problems lies at the heart of both linesearch and trust-region methods for large-scale nonlinear optimization. When there are constraints present, a typical model involves the minimization of a quadratic objective subject to linearized constraints, and perhaps a trust-region. The solution method of choice for such models is the preconditioned conjugate-gradient method, and it is now quite usual for the precondioner to respect such linearized constraints. In this talk we will describe recent work in which rather than building a preconditioner by factorizing a matrix of the correct structure (the so-called "constraint preconditioner" approach), we instead construct factors which give a preconditioner of the correct structure, based on an idea by Will Schilders. We will describe both theoretical and numerical advantages of the proposed approach. We will extend this idea to other structured systems arising from interior-point methods.

This is a joint work with Sue Dollar and Andy Wathen

Jacobian-free Optimization

Andreas Griewank
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Berlin, Germany

Classical SQP methods as well as adaptions of Interior Methods to NLP involve the forming and factoring of the active constraint Jacobian at each iteration. While this is not the case for many test problems, the cost for forming and factoring general Jacobians can be one order of magnitude more expensive than evaluating the residual. Sometimes it is impossible alltogether. Therefore we investigate one 'Total quasi-Newton' approach that approximates the Jacobian by secant updates and a 'Piggy back' approach for design optimization. The former should yield superlinear convergence, while the latter maintains at best the linear rate of a given feasibility restoration iteration.

Gradient Projection for General Quadratic Programs

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We present a new iterative method for solving large scale quadratic programs (QPs). Our approach combines a gradient projection step to identify the active constraints with an approximate solution of an equality constrained QP. The method is fully iterative and does not require any factorizations.

The gradient projection step is based on the augmented Lagrangian. The method exploits the special structure of QPs to estimate the penalty parameter, and avoids the use of arbitrary sequences usually associated with augmented Lagrangian.

The equality constrained QPs are soled inexactly by applying iterative techniques to the KKT system. We discuss an interesting connection between our approach and Newton's method applied to the first order conditions of the augmented Lagrangian. Preliminary numerical results will be presented.

This is a joint work with Michael Friedlander.

New methods for large-scale unconstrained optimization.

Ladislav Lukšan
Academy of Science of the Czech Republic,
Praha

The contribution is devoted to three classes of methods for large-scale unconstrained (or box-constrained) optimization. The first class contains so-called shifted limited-memory variable metric methods, where direction vector is determined by the formula $d = -Hg$, $H = \zeta I + A$ and A is a low-rank matrix updated by a quasi-Newton formula. These methods are globally convergent and effective for solving large-scale problems.

The second class contains variations of variable metric methods for nonsmooth optimization. The advantage of these methods is that they use small (two or three term) bundles and avoid the solution of time-consuming quadratic programming subproblems. These methods were recently used for solving large-scale nonsmooth problems.

Finally, we describe hybrid methods for large scale nonlinear least squares and efficient iterative methods for approximate solution of large-scale trust region subproblems.

This is a joint work with Jan Vlček

References: (see `http://www.cs.cas.cz/~luksan/reports.html`)

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Computing transition states: Background, theory, and computational experiments

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The mountain-pass theorem is a remarkable result that forms the basis for the calculation of transition states in biology and chemistry. The mountain-pass theorem is also a fundamental tool in nonlinear analysis where it is used to prove existence results for variational problems in infinite-dimensional dynamical systems. We describe the background for the mountain-pass theorem, and discuss algorithms for the calculation of transition states. We emphasize the elastic string algorithm.

The background needed for this presentation is minimal since we want to concentrate on the main ideas and minimize the details. We provide an overview of the convergence properties of the elastic string algorithm, and show that any limit point of the algorithm is a path that crosses a critical point. The behavior of the elastic algorithm will be examined via computational experiments for benchmark problems in infinite-dimensional variational problems.

Interior-Point and Penalty Methods for Nonlinear Programming

Jorge Nocedal
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One of the most important open questions in nonlinear interior methods is the design of adaptive strategies for updating the barrier parameter. The main goals we want to achieve are the ability to handle bad scaling and to recover from poor steps. We propose a general framework for updating barrier the parameter that guarantees global convergence, and discuss a concrete implementation. We present numerical results on difficult nonlinear programs. In the second part of the talk we study the use of penalization to handle problem degeneracies. Particular attention will be given to the interplay between the penalty and barrier terms.

Recent applications of Nash equilibria and their computations

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We discuss some recent applications of computing Nash equilibria in electric power markets (joint work with Ben Hobbs) and in multiuser digital subscriber lines (joint work with Tom Luo). These applications are studied via the theory and methods of linear and nonlinear complementarity problems. Extensions of the basic models to two-level optimization problems, which are cast as mathematical programs with equilibrium constraints (MPECs), are presented. The global solution of the latter MPECs by branch-and-cut methods is discussed and illustrated.

Multi-Quadratic 01 Programming

Panos Pardalos
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University of Florida

This presentation will focus on unconstrained and constrained quadratic 01 programming problems and their equivalent formulations. Based on these formulations we describe several linearization techniques, which allow us to solve quadratic and multi-quadratic 01 programming problems by applying any commercial package used for solving linear mixed integer programming problems. We also discuss branch-and-bound algorithms for unconstrained quadratic 0-1 programming problems, complexity issues, and applications.

The NEWUOA software for unconstrained minimization without derivatives

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Let the least value of an objective function $F(x)$, $x \in \mathcal{R}^n$, be required, where $F(x)$ can be calculated for any vector of variables x, but derivatives are not available. Experiments show that, in many cases with large n, this problem can be solved to high accuracy by the NEWUOA software of the author, using only $\mathcal{O}(n)$ values of F. On most iterations of the algorithm, a change to the variables is obtained by minimizing approximately a quadratic model, Q say, of F subject to a trust region bound, but occasionally the change to the variables is chosen to improve the accuracy of Q. Each new model has to interpolate only about $2n+1$ values of F, the remaining freedom being taken up by minimizing the Frobenius norm of the change to the second derivative matrix of Q. Thus we will find that the amount of work of an iteration is usually only $\mathcal{O}(n2)$, which allows n to be quite large. Attention will also be given to the stability of the matrix calculations that occur and to numerical results.

A Smoothing Constrained Equation Algorithm for Semi-Infinite Programming

L. Qi
The Hong Kong Polytechnic University
China

In this talk we present a new method for solving the semi-infinite programming (SIP) problem. We first reformulate the KKT system of the SIP problem into a system of constrained nonsmooth equations. Then we solve the system of equations by a smoothing projected Newton-type algorithm. Global and local superlinear convergence of this method are established under some standard assumptions. Numerical results show that the method is promising.

New Challenges in PDE-Constrained Optimization

Ekkehard W. Sachs
University of Trier
Germany

In recent years one could notice a growing interest of the community in the numerical solution and applications of optimization with partial differential equations as constraints.

The numerical cost for these problems is dominated by the effort to solve for the boundary value problems with PDEs. This puts new demands on the development of efficient optimization alogrithms.

We review several issues in this context: Reduced order models are used to lower the numerical effort for solving the PDEs and are incorporated in an optimization framework. The efficiency of the solution of the PDEs is strongly coupled to good preconditioners and we discuss how to incorporate these into the optimization solvers. Furthermore, we present several examples of PDE-constrained optimization problems in engineering and in finance.

Recent Developments for Mathematical Programs with Equilibrium Constraints

Stefan Scholtes
University of Cambridge
Cambridge, UK

Mathematical programs with equilibrium constraints (MPECs) are interesting for at least two reasons: They have immediate applications in systems design in economics and mechanics and they provide a natural benchmark for the robustness of standard NLP codes, due to their inherent ill-posedness. We review some of the advances that have been made over the past years in our understanding of the performance of either specialised or standard NLP methods for MPECs. Time permitting, we will also discuss some exciting ongoing research related to infinite dimensional MPECs or multi-player versions of MPECs, so-called equilibrium problems with equilibrium constraints (EPECs).

Multicommodity flows

J.P. Vial
University of Geneva
Switzerland

We discuss solution methods for three classes of multicommodity flow problems: linear problems, problems with fixed demands and convex congestion costs and problems with elastic demands and convex congestion costs. The solution method in the three cases is based on a proximal analytic center cutting plane method to solve a Lagrangian dual. In the linear case, the solution method is accelerated by an active set strategy. In the nonlinear case, the Lagrangian dual function inherits from the congestion function a nonlinear component that can often be given in closed form. The solution method exploits this information in the form of a single nonlinear cut, to achieve a substantial acceleration. We apply the method to the following collections of problems: the grid and the planar problems (artificial problems mimicking telecommunication networks) and real problems arising in telecommunication and traffic analysis. The largest problems in these collections are huge. We show that our solution method produces primal feasible solutions (flows) and dual feasible solution, thus a certified optimality gap.

Rapidly Convergent Algorithms for Degenerate Nonlinear Programming

Stephen Wright
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Madison, USA

We discuss techniques for nonlinear programming that achieve rapid convergence when such conditions as strict complementarity and linear independence of the active constraint gradients are not satisfied at the solution. In fact, constraint qualifications can be dispensed with altogether, provided that KKT conditions and a second-order sufficient condition hold at the solution. Identification of active constraints is a key component of the approach. We will discuss numerical aspects of the method, connections with other approaches, and applications to mathematical programs with equilibrium constraints.

Algorithms for Solving Mathematical Programs with Complementarity Constraints

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In this paper, we first point out that both bilevel programming problems (BLPP) and mathematical programs with equilibrium constraints (MPEC) can be reformulated as mathematical programs with complementarity constraints (MPCC) by replacing the lower level problem by its KKT optimal conditions. We review existing algorithms for solving MPCC and discuss their efficiency and the required assumptions to guarantee global convergence. As we know, finding a descent piece is an important subproblem in piecewise sequential quadratic programming (PSQP) algorithms for solving MPCC, and we compare the active set algorithm and the extreme point algorithm when they are used to solve this subproblem. We then propose a $\delta-$active search technique and explain its role in developing a globally convergent PSQP algorithm for solving MPCC. Numerical results for testing the new algorithm are reported. We further show that by using this technique, some algorithms for solving nonlinear programming problems can also be modified to solve MPCC.

This is a joint work with Guoshan Liu.