MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Tagungsbericht 02/2000

Continuous Optimization and Industrial Applications

(Kontinuierliche Optimierung und Industrieanwendungen)

09.01.–15.01.2000

The meeting was organized by Aharon Ben-Tal (Haifa), Arkadi S. Nemirovski (Haifa), Josef Stoer (Würzburg), and Jochem Zowe (Erlangen).

The confenence was focused on most recent topics in continuous optimization, including

- interior-point methods
- semidefinite programming
- nonsmooth optimization
- stochastic programming
- algorithms for very-large-scale nonlinear programs

Although these topics represent separate disciplines, in many ways they need each other. So this conference provided a good opportunity for the attending experts to profit from many informal discussions.

Special emphasis was given to applications of continuous optimization. Several talks showed that modern optimization methods can substantially reduce costs of industrial processes and/or speed-up the corresponding analysis.

The conference was attended by 41 participants and 34 talks were given. The pleasant atmosphere in Oberwolfach contributed to the overall succsess of the meeting.

Kurt M. Anstreicher and Nathan W. Brixius

Solution of quadratic assignment problems using continuous quadratic programming relaxations

We describe a new convex quadratic programming (QP) bound for the quadratic assignment problem (QAP). The construction of the bound uses a semidefinite programming representation of a basic eigenvalue bound for QAP. The QP bound is implemented in a complete branch-and-bound algorithm for solving QAP problems to optimality. The performance of the branch-and-bound algorithm on large, benchmark QAP problems is superior to that of previously described methods.

Alfred Auslender

Entropic proximal decomposition methods for convex programs and variational inequalities

We consider convex optimization and variational inequality problems with a given separable structure. We propose a new decomposition method for these problems which combine the recent logarithmic-quadratic proximal theory with a method of decomposition given by Chen-Teboulle for convex problems with particular structure. The resulting method allows to produce the first time provable convergent decomposition schemes based on C^∞ Lagrangians for solving structured problems. Under the only assumption that the primal-dual problems have nonempty solution sets, global convergence of the primal-dual sequences produced by the algorithm is established.

Aharon Ben-Tal, D. Falikman, E. Gordon, M. Jacobson, T. Margalit,
R. Levkovitz, and Arkadi Nemirovski

Convex optimization in nuclear tomography

We describe an optimization problem arising in reconstructing 3D medical images from Positron Emission Tomography (PET). A mathematical model of the problem, based on the Maximum Likelihood principle is posed as a problem of minimizing a convex function of several millions variables over the standard simplex. To solve a problem of these characteristics, we develop and implement a new algorithm, Ordered Subsets Mirror Descent, and demonstrate, theoretically and computationally, that it is well suited for solving the PET reconstruction problem.

Martin Bendsøe

Algorithms in structural optimization: looking ahead (back)

In structural optimization one works with state variables and design (control) variables. The typical optimization problem can be formulated in both variables, indicating that the solution of the design to state relation is viewed as a constraint (can be an equation or some variational problem). This will then mean that solving a finite element problem is part of the optimization. This approach has been very successful for very specific classes of problems, such as minimum compliance truss design where a unique problem structure allows for a convex formulation as for example a SDP. However, the standard procedure is to view the state equation—which can involve calling a huge finite element code—as a function call with associated derivatives computed through sensitivity analysis, an area of engineering interest in its own right. Sequential linear and quadratic programming algorithms have seen widespread use for solving the non-convex problem in the design variables only, but the most popular methods are based on *convex, separable* approximations (CONLIN, MMA). The future calls for work on stable general purpose algorithms for large scale computations, use of response surface and surrogate modelling techniques for 'noisy' problems and the possible application of multigrid method seems to be an interesting approach which uses the origin of the problems, namely as distributed parameter "control" problems.

Francisco Facchinei

Newton method for nonsmooth equations

We consider the equation $F(x) = 0$, where $F : \mathbb{R}^n \to \mathbb{R}^n$ is assumed to be locally Lipschitz, and wish to design a local, superlinear method for its solution. To this end we consider iterations $x^k + d^k = x^{k+1}$ where d^k is the solution of a "Newton" equation of the type $F(x^k) + A(x^k, d) = 0$. Under appropriate assumptions on the term $A(x, \cdot)$, we show that the resulting method is well defined and locally superlinearly/quadratically convergent. Finally we show that the resulting scheme allows us to recover practically all the Newton schemes proposed up to now in the literature.

Sharon Filipowski

Applications of nonsmooth optimization in industry

A number of applications of nonsmooth optimization in industry are discussed. Particular focus is given to the use of nonsmooth optimization when addressing the solution of combinatorial optimization problems using the method of Lagrangian relaxation. The application discussed in this area is the Data Association Problem that arises in multitarget tracking. In addition, applications of semidefinite programming including model tuning problems arising in the analysis of aircraft structures, matrix scaling problems arising in a number of applications, and graph partitioning problems are discussed.

Andreas Fischer

On the local behavior of an algorithmic framework for generalized equations

An algorithmic framework for solving generalized equations with not necessarily isolated solutions will be presented. General conditions will be given that ensure local superlinear convergence of algorithms within this framework. Applied to particular generalized equations (NCP or KKT conditions, for instance) the approach leads to new ideas and results as well as to a new understanding of existing convergence theories.

Roger Fletcher

Filter methods in nonlinear programming (NLP)

Filter methods provide an alternative to penalty function methods in globalizing algorithms for NLP. Filter methods are based on the dominance principle of multi-objective optimization and provide a criterion for accepting or rejecting a step in an iterative method.
Some issues in applying a filter to a trust region SQP method are considered. The possibility that infeasible QP subproblems are generated is handled by the introduction of a "feasibility restoration" phase. Strategies for avoiding filter entries which block progress to a solution are described. Numerical experience is very satisfactory.
The possibility of making a global convergence theory is discussed in the context of SLP. Some minimal heuristics are suggested which enable convergence to a Fritz-John point to be proved.

Robert M. Freund

Geometry and the complexity of the convex feasibility problem

Many researchers have analyzed the complexity of finding a point in a convex set, suitably described, in terms of a variety of condition numbers and/or other complexity parameters, including the data-based condition number of Renegar, the Todd-Stewart measure relating a certain subspace to the coordinate suborthants, Ye's measure σ, and the bit-length L of the data, for example. In this talk we purposely abandon all of these measures in favor a geometric measure involving the extent to which the feasible region contains a ball that is not too small and not too far from a given reference point, say the origin. Let us call this measure g, for geometry measure. We show that there are versions of both interior-point algorithms and ellipsoid-type algorithms for finding a point in a convex set whose complexity is bounded above by a function proportional to $\ln(g)$. We also show that this dependence cannot be structurally eliminated for the ellipsoid algorithm. Finally, we show how to compute an approximation of g as part of an algorithm for finding a point in a convex set.

Osman Güler

Hyperbolic polynomials and convex analysis

During the last hundred years, many results have been obtained concerning eigenvalues of symmetric matrices and singular values of general matrices. Some of these problems are convex optimization problems which can be solved efficiently using semidefinite programming.
We show that many of these results can be obtained from a unified point of view using the concept of hyperbolic polynomials. We then show that hyperbolic polynomials help extend these results to many different applications. Finally, we indicate some open problems and further avenues for research.

Christoph Helmberg

A spectral bundle method with bounds

Semidefinite relaxations of quadratic 0-1 programming or graph partitioning problems are well known to be of high quality. However, solving them by primal-dual interior point methods can take much time even for problems of moderate size. The recent spectral bundle method of Helmberg and Rendl can solve quite efficiently large structured equality-constrained semidefinite programs if the trace of the primal matrix variable is fixed, as happens in many applications. We extend the method so that it can handle inequality constraints without seriously increasing computation time. Encouraging preliminary computational results are reported.

Herbert R.E.M. Hörnlein and M. Stettner

Structural design process: projects–programs–prospects

The structural design process is traditionally divided into three phases, each of which poses characteristic questions to the designer. Typical optimization problems in conceptual, preliminary and detailed design are described, existing methods for their solution are reviewed, and an outlook of future developments is presented. Three examples are briefly discussed to show the applicability of existing structural optimization software. The significance of mathematical programming as a driver for the solution of contemporary, challenging problem statements is outlined. The transition between phases, models, and methods is identified as a current pitfall of the design process as a whole. A brief overview of Multi-Disciplinary Optimization (MDO) techniques shows how these methods primarily support the preliminary and detailed design phase. Conceptual design is intentionally emphasized due to its lack of MDO support and potential within the design process. It is concluded that interdisciplinary cooperation, specifically between engineers and mathematicians, is the key to future improvement.

Florian Jarre

A primal interior-point method for nonconvex minimization

In several applications, semidefinite programs with nonlinear equality constraints or bilinear semidefinite programs arise. In both cases, the optimization problem is no longer convex. We

propose a new solution method for smooth nonconvex programs that is based on a primal barrier method. Primal predictor corrector logarithmic barrier methods are known to be efficient—in theory as well as in practice—for solving convex semidefinite programs. The key observation for the theoretical analysis of a primal barrier method for solving convex semidefinite programs is a local Lipschitz continuity (self-concordance) of the Hessian of the logarithmic barrier function. We motivate why it seems very difficult to generalize the concept of self-concordance to nonconvex functions. Nevertheless one can anticipate that the continuity properties of the Hessian of the logarithmic barrier function are not lost completely when the problem involves nonconvex components.
The global analysis of Newton's method for self-concordant minimization relies on a "trust region interpretation" of Newton's method. The shape of the trust region is naturally given by the ellipsoid defined by the Hessian of the barrier function. This convex trust region is affine invariant, and on the boundary of the trust region, the deviation of the barrier function from its linearization is approximately constant. It is easy to show that both properties cannot be maintained in the nonconvex case, and thus, the choice of a suitable trust region is less evident.
We generalize Newton's method to a trust region method with two parameters controlling the step length and the shape of the trust region, and we discuss the arithmetic costs for this approach.
The predictor steps are based on Dikin-ellipsoids of a "convexified" domain.
Some convergence results are given, and some preliminary but promising numerical experiments suggest a high robustness of the proposed method.

Christian Kanzow

Smoothing-type methods for linear programs

Smoothing-type methods for the solution of linear programs are closely related to the class of primal-dual path-following methods. In fact, they also try to follow a certain path, typically called the smoothing path. In some situations, this smoothing path coincides with the central path known from the interior point literature. In contrast to primal-dual path-following methods, however, smoothing-type methods do not require all iterates to stay (strictly) feasible. The main idea of several smoothing-type methods will be discussed in detail, together with their theoretical and numerical properties.

Krzysztof C. Kiwiel, T. Larsson, and P.O. Lindberg

Dual properties of ballstep subgradient methods

We study the recent subgradient projection methods for convex optimization that use ballstep level controls for estimating the optimal value. Via averaging, they asymptotically find optimal objective subgradients and constraint multipliers. Applied to Lagrangian decomposition of convex programs, they find both primal and dual solutions, and have practicable stopping criteria. We give numerical results for several large-scale applications, including traffic assignment and message routing in networks.

Michal Kočvara

Structural optimization with stability constraints

The goal of the talk is to find a computationally tractable formulation of the optimum truss design problem involving a constraint on the global stability of the structure. The stability constraint is based on the linear buckling phenomenon. We formulate the problem as a nonconvex semidefinite programming problem and briefly discuss an interior point technique for the numerical solution of this problem. We further discuss relation to other models. The talk is concluded by a series of numerical examples.

Bernd Kummer

Newton methods for KKT-points: resulting problems depending on the type of approximation

Newton-type methods for finding KKT-points of C^2 (and less smooth) problems

$$\min f(x) \text{ s.t. } g(x) \leq 0$$

(in finite dimension) can be applied to the perturbed (by $t \neq 0$) Kojima equation $F^t(x,y) = 0$, where

$$F_1^t = Df(x) + \sum y_i^+ Dg_i(x) \qquad \text{and} \qquad F_{2i}^t = g_i(x) - y_i^- - t_i y_i^+.$$

Other approaches use so called NCP-functions $G : \mathbb{R}^2 \to \mathbb{R}$ with $G^{-1}(0) = \{(u,v) \geq 0 \mid uv = 0\}$ and equivalent system $\Phi(x,y) = 0$, which stands for $D_x L(x,y) = 0$, $G(-g_i(x), y_i) = 0$. In these cases, Newton steps use certain generalized derivatives at non-C^1 points of F^t or Φ. We compare them for generalized Jacobians applied to F^t and so-called B-derivatives applied to G. As a result we obtain for any positively homogeneous G being PC^1 on the sphere:

A Newton step at (x,y) means to find a KKT-point (u,μ) of a problems

$$P(r) \qquad \begin{array}{l} \min\limits_u (Df + \sum\limits_{k \in K} y_k\, Dg_k)u + \frac{1}{2} u^T D_x^2 L u + \frac{1}{2} \sum\limits_{i \in J} w_i (g_i + Dg_i\, u)^2 \\ s.t. \qquad g_k + Dg_k\, u = 0 \qquad \text{for all } k \in K \end{array}$$

where $w_i = r_i b_i^{-1}$, and v is uniquely defined by u and μ.

In case 1, r may be any fixed vector satisfying $r_i \in [0,1]$ and $r_i = 0$ (if $y_i < 0$) and $r_i = 1$ (if $y_i > 0$), $b_i = 1 - r_i - t_i r_i$, and $K = \{k \mid b_k = 0\}$, $J = \text{compl}(K)$. So P(r) depends on t, too.

In case 2, now (r_i, b_i) takes the place of $DG(-g_i(x), y_i)$ or, if G is not C^1 around the argument, (r_i, b_i) is any limit of $DG(p)$ for p tending to $(-g_i(x), y_i)$ in the C^1-region of G. The derivatives of the Lagrangian L are taken at (x, y^+) and (x,y), respectively. In both cases (and for $t = 0$), the Newton methods (locally superlinear) converge iff—at the solution (x^*, y^*)—all the problems P(r) have only the trivial KKT-point. Using F, this means strong regularity in Robinson's (1980) sense. Using Φ with "sufficiently smooth" G, one obtains the same requirement. Having this, the zeros of F^t for $t_i > 0$ ($t_i < 0$) yield critical points of the penalty (barrier) functions which can be Lipschitzian estimated each other for small norm of t (even if the signs are not the same). So, setting $t = t(x,y)$ at each Newton step and organizing $t \to 0$ sufficiently fast (estimates are given), Newton steps realize second order steps in quadratic approximations assigned to (mixed) Penalty-Barrier methods and can model (in particular) the Newton steps assigned to Φ.

Claude Lemaréchal

Lagrangian duality & SDP relaxation for combinatorial optimization

We show that it is fruitful to dualize the integrality constraints in a combinatorial optimization problem. First, this reproduces the known SDP relaxations of the max-cut and max-stable problems. Then we apply the approach to general combinatorial problems. We show that the resulting duality gap is smaller than with the classical Lagrangian relaxation; we also show that linear constraints need a special treatment.

Sven Leyffer

Filter methods for nonsmooth optimization

We consider minimizing a nonsmooth objective subject to nonsmooth constraints. The nonsmooth functions are approximated by a bundle of subgradients. The novel idea of a filter is used to promote global convergence.

Yuri Nesterov

Stochastic programming: Any guarantees in the uncertain world?

We propose an alternative approach to stochastic programming based on Monte-Carlo sampling and stochastic gradient optimization. The procedure is by essence probabilistic and the computed solution is a random variable. The associated objective value is doubly random, since it depends on two outcomes: the event in the stochastic program and the randomized algorithm. We propose a solution concept in which the probability that the randomized algorithm produces a solution with an expected objective value departing from the optimal one by more than ϵ is small enough. We derive complexity bounds for this process. We show that by repeating the basic process on independent sample, one can significantly sharpen the complexity bounds.

Jiří Outrata

Second-order subdifferentials and their application in variational systems

For a special class of nonsmooth functions we provide formulas enabling the computation of their 2nd-order Mordukhovich's subdifferentials or upper approximations of these sets. These subdifferentials can well be used in the stability and sensitivity analysis of variational inequalities and complementarity problems. Furthermore, they play an important role in so-called mathematical programs with equilibrium constraints with respect to optimality conditions and numerical methods. Examples will be given, illustrating the application of the presented theory to some problems of continuum mechanics.

Jong–Shi Pang

Mathematical programs with equilibrium constraints

Mathematical Programs with Equilibrium Constraints are constrained optimization problems which contain a parametric variational inequality as part of he contraints. We discuss the application of these problems to inverse optimization and inverse pricing of equilibrium systems. We also present some details of one such application to the computation of an implied volatility surface in the pricing of American options.

Josef Stoer and <u>Martin Preiß</u>

High-order interior-point methods for solving LCP's

In our talk we are concerned with methods for solving linear complementarity problems (LCP) that are monotone or at least sufficient in the sense of Cottle, Pang and Venkateswaran (1989). A basic concept of interior-point methods is the concept of (perhaps weighted) feasible or infeasible interior-point paths. They converge to a solution of the LCP if a natural path parameter, usually the current duality gap, tends to zero.
It is shown how the analyticity properties of these paths can be used to devise long-step path-following methods for which the duality gap converges Q-superlinearly to zero with an arbitrary high order $p+1-\varepsilon$ (resp. $(p+1)/2-\varepsilon$) if the LCP has strictly complementary (resp. no strictly complementary) solutions and certain infeasible interior-point paths are approximated by polynomial of degree p.

<u>Franz Rendl</u> and K. Kunisch

An infeasible active set method for convex problems with simple bounds

We propose a new active set method, where in each iteration, the new active set is determined from scratch. We give sufficient conditions for finite termination of this approach and provide pratical experiance, indicating that this method is highly competitive with other approaches for this type of problems.

Stephen M. Robinson and Richard R. Laferriere

Scenario analysis in U.S. Army decision making

We describe a ten-year project that has changed the way in which the U.S. Army conducts force analysis and design. The underlying methodology consists of a stochastic time-staged linear programming model, implemented using combat simulations, together with a decision support system for interacting with senior managers who must use the results of the analysis.

Kees Roos

A new polynomial large-update primal-dual method for linear optimization

It is now known that interior-point methods (IPMs) for linear optimization (LO) that use small updates of the barrier parameter μ admit an $O(\sqrt{n}\log\frac{n}{\varepsilon})$ iteration bound, whereas methods that use large updates have a worse iteration bound, namely $O(n\log\frac{n}{\varepsilon})$. Here n denotes the dimension of the problem. Contrary to these theoretical results, large-update IPMs work much more efficient in practice than small-update IPMs. To close this gap between the theory and practice, several authors showed that the complexity of large-update IPMs can be improved by using high-order versions of the "classical" primal-dual Newton search direction. We propose a new primal-dual search direction for linear optimization. By using some new tools in the analysis we obtain a large-update method that admits an $O\left(n^{\frac{2}{3}}\log\frac{n}{\varepsilon}\right)$ iteration bound, thus partially closing the above mentined gap. Just as for the usual Newton direction, at each iteration only one linear eqaution system has to be solved. An extension of the results to semidefinite optimization is almost straightforward.

Ekkehard Sachs

Optimization methods in food sterilization

Mathematical methods gained significant importance in the field of food processing in recent years. The modeling of food sterilization is much improved and the technology is available to make strategies developed with optimization methods applicable in the food industry. We formulate several problems from industry in mathematical terms as optimzation problems which grew out of cooperation with industry. As an example we consider the optimal control of heating for maximal retention of vitamines under the fulfilment of sterilization. This leads to an optimal control problem which itself lends a large scale optimization problem when discretized properly. We show how SQP methods can be applied in this context and interpret the final results for the model in terms of the industrial application.

Klaus Schittkowski

Computer aided optimal design of horn radiators for satellite communication

The intention of the paper is to outline a mathematical model for designing high performance circular corrugated horns using an optimization algorithm. The proposed approach is based on an analytic computation of the electromagnetic field in the aperture that generates a given far field. In a subsequent step, the inner geometry of a corrugated horn is adjusted by an optimization algorithm (sequential quadratic programming) to generate the aperture field. For the computation of the electromagnetic fields an analysis routine of Kühn and Hombach is applied. The method has been successfully applied to design corrugated horns which radiate a given directional field pattern.

Johannes Schloeder

Numerical methods for parameter estimation and optimum experimental design in nonlinear differential equations

Modelling of complex dynamic processes is a difficult and time consuming procedure that requires the solution of challenging optimization problems at several stages. The talk formulates typical optimization problems and describes recent numerical methods for their solution.
Emphasis is laid on Boundary Value Problem Methods for parameter estimation in large-scale differential algebraic equation systems and on direct approaches for the solution of state constraint optimal control problems arising in nonlinear optimum experimental design.
Industrial applications of the methods including chemical reaction kinetics and transport and degradation processes for xenobiotica in soil are discussed.

Stefan Scholtes

Measuring the robustness of empirical efficiency valuations

The technique of data envelopment analysis (DEA) allows the evaluation of the efficiency of a production process relative to competing precesses. The technique is based on input and ouput data of a sample of production processes and assigns to each of the sampled processes a relative efficiency score between zero and unity where a unit score indicates relative efficiency of the process among the group of sampled processes. The score—or rather one minus the score—of an *inefficient* process can be interpreted as a robustness measure for an empirical efficiency valuation with respect to perturbations of a particular subset of the sampled data and a particular metric. We will argue that the admissible perturbations and/or metric of standard DEA appears rather *ad hoc* and may lead to arguable results in practical applications. To remedy this drawback we suggest a more general model for structured robustness measure which encompasses DEA efficiency scores as special cases. It turns out that this model is close in spirit to Renegar's condition number for linear inequality systems.
While the standard DEA efficiency score of a process can be calculated by solving linear program, the computation of a more general rubustness measure is typically more difficult and involves the global solution of a nonconvex optimization problem. It turns out, however, that this computation is tractable in a variety of practical relevant cases. A capacity planning problem for hospitals is used to illustrate the applicability of the research. The talk is based on joint work with Ludwig Kuntz of the University Hospital at Hamburg.

A. Kaplan and Rainer Tichatschke

Auxiliary problem principle and proximal point method

An extension of the auxiliary problem principle to variational inequalities with non-symmetric multi-valued operators in Hilbert spaces is studied. This extension supposes that the operator of the variational inequality is splitted into the sum of a maximal monotone operator Q and a single-valued operator $\mathcal{F}$, and $\mathcal{F}$ is linked with a sequence $\{\mathcal{L}^k\}$ of non-symmetric components of auxiliary operators by a kind of pseudo Dunn-property. The current auxiliary problem is constructed by fixing $\mathcal{F}$ at the previous iterate, whereas Q (or its single-valued approximation Q^k) is considered at a variable point. Using auxiliary operators of the form $\mathcal{L}^k + \chi_k \nabla h$, with $\chi_k > 0$, the standard for the auxiliary problem principle assumption of the strong convexity of h is weakened by exploiting mutual properties of Q and h. Convergence of the general scheme is analyzed allowing that the auxiliary problems are solved approximately, and some applications (long-step decomposition methods, non-smooth optimization problems, contact problems with friction) are sketched briefly.

Michael Todd and E. Alper Yildirim

Sensitivity analysis for linear and semidefinite programs

We analyze perturbations of the right-hand side and the cost parameters in linear programming (LP) and semidefinite programming (SDP). We obtain tight bounds on the perturbations that allow interior-point methods to recover feasible and near-optimal solutions in a single interior-point iteration. For the case of a unique, non-degenerate solution in LP, we show that the bounds obtained using an interior-point method compare nicely with the bounds arising from the simplex approach. We also present explicit bounds for SDP using the AHO, HRVW/KSH/M, and NT directions.

Philippe Toint, A. Conn, N. Gould, and D. Orban

Primal-dual methods for general nonlinear programming

The talk will describe a primal-dual algorithm for solving nonlinear optimization problems with inequality or linear equality constraints. No convexity assumption is made on the objective function or constraints. The algorithm itself will be described, as well as some preliminary numerical experience. The talk will also present the growing body of convergence analysis related to the algorithm, including global convergence to points satisfying second-order criticality conditions and an analysis of the local rate of convergence under nondegeneracy assumptions.

Robert J. Vanderbei

Interior-point methods for second-order-cone and semidefinite programming

Interior-point methods for smooth convex nonlinear programming (NLP) problems involve simple extensions of the corresponding algorithm for linear programming. In particular, the nonnegative orthant is the fundamental cone on which the algorithm is based. For second-order-cone programming (SOCP) and semidefinite programming (SDP) the fundamental cone is different. Namely, it is the Lorentz cone and the cone of semidefinite matrices, respectively. In this talk, we address how to reformulate SOCPs and SDPs so that they can be solved with an interior-point method for smooth convex NLP. We then present computational results illustrating the effectiveness of this approach using a specific interior-point code for NLP.

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