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FINAL TECHNICAL REPORT

to Air Force Office of Scientific Research

"Numerical Methods of Linear and Nonlinear Optimization"

Grant Number AFOSR 87-0215

Accomplishments: July 1, 1987 - September 30, 1991

March 3, 1992

David F. Shanno Principal Investigator



Abstract

The project has been concerned with developing new numerical techniques to solve large scale linear and nonlinear programming problems. Early work focused on sequential quadratic programming techniques for nonlinear programming. Subsequently, all work was focused on interior point methods for large scale linear and nonlinear programming. Initially, the focus of the research was dual-affine and primal-dual algorithm for linear on both Substantial computational experience demonstrated programming. the superiority of the primal-dual methods, and subsequent research focused on improving the efficiency of these methods, both by adding higher order methods via predictor-corrector techniques and by improving the linear algebra to take advantage of both sparsity and machine architecture. Most recently, research has focused on large scale quadratic programming. A primal-dual predictor-corrector method has been devised and shown to be very promising computationally for problems with diagonal or sparsely structured Hessian matrices. For problems with dense Hessians, a pure primal conjugate projected gradient algorithm shows promise on small problems. It remains to be tested on large-scale problems.

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5. Abstracts of Technical Papers

Summary of Research Accomplishments

The initial research undertaken under the grant was a numerical study of various topics in sequential quadratic programming. The topics studied included Lagrange multiplier estimates, choice of merit function, choice of search direction, and choice of penalty parameter. Extensive testing determined a stable algorithm for the standard test set, and indicated the need for further research in multiplier estimates, research which will be undertaken in the next year.

All other research throughout the duration of the grant was concerned with interior point methods for linear and nonlinear programming. Initially, research into developing a viable computational algorithm took two separate directions, a full scale implementation of a dual affine algorithm and a prototype implementation of a primal-dual algorithm. The dual-affine implementation served as an interesting platform for devising algorithms for bounded variables, eliminating rows and columns, testing starting points, and for examining the importance of centering.

The prototype studies of the primal-dual algorithm demonstrated that the method had great computational promise, and was far more stable than the dual affine algorithm. Analysis demonstrated that this stability was largely due to the automatic centering of the algorithm. In view of this, implementation of a full scale primal-dual algorithm was undertaken. This implementation proved so satisfactory that all further research for linear programming concentrated on this algorithm.

Work on the prototype algorithm had demonstrated how to incorporate bounded variables and ranges into the algorithm. Early work on the full implementation of the original algorithm focused on improved algorithms for choice of the centering parameter, better initial estimates to the solution, and better ways to find feasible solutions. A major breakthrough in handling infeasibility occurred when Newton's method was applied directly to the first order necessary conditions from an infeasible starting point. This method has proved highly successful in practice, and remains the standard way of handling infeasibility.

A great deal of research dealt with the problem of special handling of dense columns in the constraint matrix. These columns can make the Cholesky factorization of the matrix of normal equations unacceptably dense, but this problem can be overcome by careful special handling. While reasonable techniques to handle dense columns have been implemented, the problem remains one for further study. The next major advance in the linear programming algorithm came with the implementation of higher-order methods via the predictor-corrector technique. In addition to implementing the predictor-corrector method, which reduced run time by approximately 40%, research concentrated on analyzing the method and investigating higher-order predictor-corrector methods. While higher-order methods proved theoretically interesting, a single corrector term has proved computationally the most efficient algorithm.

Further speedups of the algorithm came from improving the numerical linear algebra. Incorporation of supernodes and loop unrolling improved speed up to 40% on large problems. Further tailoring the choice of matrix ordering algorithm and Cholesky factorization to specific architectures significantly improved solution times. Research continues on improvements in this area, particularly on matrix orderings.

More recent research has concentrated on applying interior point methods to nonlinear programming problems. Initial research concentrated on applying straight primal-dual and primal-dual predictor-corrector algorithms to separable quadratic programming problems. Computational results even extremely encouraging, and have led to further research in two areas: nonseparable problems with sparse Hessian matrices and nonseparable large-scale problems with dense Hessian matrices. Primal-dual predictor-corrector algorithms have been successfully implemented for sparse Hessians. However, if the Hessian is large and dense, factorizing the matrix can become highly inefficient.

To attack problems with large dense Hessians, but hopefully multiple clustered eigenvalues, a primal algorithm based on conjugate projected gradients has been devised and tested in a prototype version. Computational results are sufficiently encouraging that work is currently underway to develop a full blown code for large problems.

Finally, when acceptable algorithms for quadratic programming have been fully developed, these will be incorporated as the quadratic programming algorithm in a sequential quadratic programming method for nonlinear programming. Thus during the next phase of the research, the topic will come full circle back to the original study on sequential quadratic programming, but with the capability of solving far larger problems than when the research was initiated.

Articles Published

- 1. D.F. Shanno, "Computing Karmarkar Projections Quickly," <u>Math</u> <u>Programming</u> 41, 1988, pp. 61-71.
- 2. D.F. Shanno and K.H. Phua, "Numerical experience with sequential quadratic programming algorithms for equality constrained nonlinear programming," <u>Trans. on Math. Software</u> 15, 1989, pp. 49-63.
- 3. K.A. McShane, C.L. Monma and D. Shanno, "An implementation of a primal-dual interior point method for linear programming," <u>ORSA Journal on Computing</u> 1, 1980, pp. 70-83.
- 4. R.E. Marsten, M.J. Saltzman, D.F. Shanno, G.S. Pierce and J.F. Ballintijn, "Implementation of a dual affine interior point algorithm for linear programming," <u>ORSA Journal on Computing</u> 1, 1989, pp. 287-297.
- 5. D.F. Shanno and A. Bagchi, "A unified view of interior point methods for linear programming," <u>Annuals of Operations</u> <u>Research</u> 22, 1990, pp 55-70.
- 6. I.C. Choi, C.L. Monma, and D.F. Shanno, "Further Development of a primal-dual interior point method," <u>ORSA Journal on</u> <u>Computing</u> 2, 1990, pp 304-311.
- 7. I.J. Lustig, R.E. Marsten, and D.F. Shanno, "Computational experience with a primal-dual interior point method for linear programming," <u>Journal of Linear Algebra and</u> <u>Applications</u> 152, 1991, pp. 191-222.
- I.J. Lustig, Re.E. Marsten, and D.F. Shanno, "The primaldual interior point method of the CRAY supercomputer," <u>Large</u> <u>Scale Numerical Optimization</u>, T. Coleman, ed., SIAM, 1990, pp. 70-80.

Articles Accepted

- 1. T.J. Carpenter, I.J. Lustig, J.M. Mulvey and D.F. Shanno, "Separable quadratic programming via a primal-dual interior point method and its use in a sequential procedure," <u>ORSA</u> <u>Journal on Computing</u> (in press).
- 2. I.J. Lustig, R.E. Marsten, and D.F. Shanno, "On implementing Mehrotra's predictor-corrector interior point method for linear programming," <u>SIAM Journal on Optimization</u> (in press).
- 3. I.J. Lustig, R.E. Marsten, and D.F. Shanno, "The interaction of algorithms and architectures for interior point methods," <u>Advances in Optimization and Parallel Processing</u>, P. Pardalos, ed., North Holland (in press).
- 4. R.E. Bixby, J.W. Gregory, I.J. Lustig, R.E. Marsten and D.F. Shanno, "Very large-scale linear programming: A case study in combining interior point and simplex methods," <u>Operations Research</u> (in press).
- 5. T.J. Carpenter, I.J. Lustig, J.M. Mulvey, and D.F. Shanno, "Higher order predictor-corrector interior point methods with application to quadratic objectives," <u>SIAM Journal on</u> <u>Optimization</u> (in press).

Articles Under Review or Revision

- 1. I.J. Lustig, R.E. Marsten, and D.F. Shanno, "Starting and restarting the primal-dual interior point method," RRR #61-90, RUTCOR, Rutgers University, New Brunswick, NJ, October, 1990.
- 2. T.J. Carpenter and D.F. Shanno "An interior point method for quadratic programs based on conjugate projected gradients," RRR #55-91, RUTCOR, Rutgers University, New Brunswick, NJ, October 1991.

Talks Presented at Meetings (All talks were invited)

Workshop on Optimization on Supercomputers, University of Minnesota, Minneapolis, May 1988.

Conference on Optimization, Mathematics Research Institute, Oberwolfach, W. Germany, January 1988.

ORSA/TIMS National Meeting, Washington, D.C., April 1988.

Mathematical Programming Society International Meeting, Tokyo, Japan, Sept. 1988.

SIAM Conference on Optimization, Boston, MA, April 1989.

ORSA National Meeting, Vancouver, B.C., May 1989.

IBM European Institute, Garmisch Partenkirchen, W. Germany, July 1989.

ORSA/TIMS National Meeting, New York, October 1989.

SIAM Conference on Large Scale Numerical Optimization, Cornell University, October 1989.

Oberwolfach Conference on Optimization, Oberwolfach, West Germany, January 1990.

Asilomar Conference on New Directions in Linear Programming, Monterey, CA, February 1990.

SIAM National Meeting (Plenary talk), Chicago, July 1990.

TIMS College of Management Practice, Hofstra University, August 1990.

ORSA/TIMS National Meeting, Philadelphia, October 1990.

APMOD91 (Applied Mathematical Programming and Modelling), London, England, January 1991, (Plenary talk).

Optimization Days, Montreal, Canada, May 1991, (Plenary talk).

ORSA/TIMS National Meeting, Nashville, TN, May 1991.

IMACS Congress, Dublin, Ireland, July 1991.

Conference on Large Scale Optimization, Coimbra, Portugal, July 1991.

Mathematical Programming Symposium, Amsterdam, Netherlands, August 1991, (Plenary talk).

IFORS Congress, Zurich, Switzerland, September 1991.

<u>Award</u>

The E.M.L. Beal-W.B. Orchard-Hays Prize for Excellence in Computational Mathematical Programming, Mathematical Programming Society, 1991, won jointly with I.J. Lustig and R.E. Marsten.

<u>Abstracts</u>

"The Primal-Dual Interior Point Method on the Cray Supercomputer"

This paper discusses computational experience on the Cray Y-MP supercomputer with the primal-dual interior point code OB1. Results are given for a variety of medium to large size models with comparisons to workstation implementations and published results for the KORBX System. Empirical results on the growth of the iteration count with the number of variables are given and areas for future research are discussed.

"On Implementing Mehrotra's Predictor-Corrector Interior Point Method for Linear Programming"

Mehrotra recently described a predictor-corrector variant of the primal-dual interior point algorithm for linear programming. This paper describes a full implementation of this algorithm, with extensions for solving problems with free variables and problems with bounds on primal variables. Computational results on the NETLIB test set are given to show that this new method almost always improves the performance of the primal-dual algorithm and that the improvement increases dramatically as the size and complexity of the problem increases. A numerical instability in using Schur complements to remove dense columns is identified, and a numerical remedy is given.

"Higher Order Predictor-Corrector Interior Point Methods with Application to Quadratic Objectives"

In this paper, we explore the full utility of Mehrotra's predictor-corrector method in the context of linear and convex quadratic programs. We describe a procedure for doing multiple corrections at each iteration and implement it within the framework of several strategies for determining the number of corrections in a given iteration. The results indicate the iteration counts can be significantly reduced by allowing higher order corrections but at the cost of extra work per iteration. The procedure is shown to be a level-m composite Newton interior point method where m is the number of corrections performed in an iteration. "The Interaction of Algorithms and Architectures for Interior Point Methods"

This paper examines the minimum local fill-in and multiple minimum degree reordering strategies for sparse positive definite symmetric systems of equations arising from interior point methods for linear programming. The performance of each ordering strategy is studied with both leftward and rightward looking sparse Cholesky decompositions utilizing supernode and loop unrolling techniques. The various algorithms are tested on a DECstation 3100, ... IBM RISC/System 6000 Powerstation 530, and CRAY Y-MP. Computational results are given to show that the correct choice of algorithm is hardware dependent.

"Separable Quadratic Programming via a Primal-Dual Point Method and its use in a Sequential Procedure"

This paper extends a primal-dual interior point procedure for linear programs to the case of convex separable quadratic objectives. Included are efficient procedures for: attaining primal and dual feasibility, variable upper bounding, and free variables. A sequential procedure that invokes the quadratic solver is proposed and implemented for solving linearly constrained convex separable nonlinear programs. Computational results are provided for several large test cases from stochastic programming. The proposed methods compare favorably with MINOS, especially for the larger examples. The nonlinear programs range in size up to 8700 constraints and 22000 variables.

"Very Large-Scale Linear Programming: A Case Study in Combining Interior Point and Simplex Methods"

Experience with solving a 12,753,313 variable linear program is described. This problem is the linear programming relaxation of a set partitioning problem arising from an airline crew scheduling application. A scheme is described that requires successive solutions of small subproblems, yielding a procedure that has little growth in solution time in terms of the number of Experience using the simplex method as implemented in variables. CPLEX, an interior point method as implemented in OB1, and a hybrid interior point/simplex approach is reported. The resulting procedure illustrates the power of an interior point/simplex combination for solving very large-scale linear programs.

"Numerical Experience with Sequential Quadratic Programming Algorithms for Equality Constrained Nonlinear Programming"

Computational experience is given for a sequential quadratic programming algorithm when Lagrange multiplier estimates, Hessian approximations, and merit functions are varied to test for computational efficiency. Indications of areas for further research are given.

"Computing Karmarkar Projections Quickly"

The paper presents a numerical method for computing the projections for Karmarkar's new algorithm for linear programming. The method is simple to implement, fully exploits sparsity, and appears in limited experimentation to have good stability properties. Preliminary numerical experience indicates that the method promises advantages over methods that refactor a matrix at every iteration.

"A Unified View of Interior Point Methods for Linear Programming"

The paper shows how various interior point methods for linear programming may all be derived from logarithmic barrier methods. These methods include primal and dual projective methods, affine methods, and methods based on the method of centers. In particular, the paper demonstrates that Karmarkar's algorithm is equivalent to a classical logarithmic barrier method applied to a problem in standard form.

"Implementation of a Dual Affine Interior Point Algorithm for Linear Programming"

The dual affine interior point method is extended to handle variables with simple upper bounds as well as free variables. During execution, variables which appear to be going to zero are fixed at zero, and rows with slack variables bounded away from zero are removed. A variant of the big-M artificial variable method to attain feasibility is derived. The simplex method is used to recover an optimal basis upon completion of the algorithm, and the effects of scaling are discussed. Computational experience on a variety of problems is presented. "An Implementation of a Primal-Dual Interior Point Method for Linear Programming"

The purpose of this paper is to describe in detail an implementation of a primal-dual interior point method for solving linear programming problems. Preliminary computational results indicate that this implementation compares favorably with a comparable implementation of a dual affine interior point method, and with MINOS 5.0, a state-of-the-art implementation of the simplex method.

"Further Development of a Primal-Dual Interior Point Method"

The paper continues the development of a primal-dual interior point algorithm for linear programming. The topics studied include simple bounds on primal variables, incorporation of Lustig's phase 1 algorithm and the use of Schur complements to handle dense columns. Extensive numerical results demonstrate the efficiency of the resulting algorithm.

"Computational Experience with a Primal-Dual Interior Point Method for Linear Programming"

new comprehensive implementation of a primal-dual It allows for Α algorithm for linear programming is described. easy handling of simple bounds on the primal variables and incorporates free variables, which have not previously been included in a primal-dual implementation. We discuss in detail a variety of computational issues concerning the primal-dual implementation and barrier methods for linear programming in general. We show that, in a certain way, Lustig's method for obtaining feasibility is equivalent to Newton's method. This demonstrates that the method is in some sense the natural way to reduce infeasibility. The role of the barrier parameter in computational practice is studied in detail. Numerical results are given for the entire expanded NETLIB test set for the basic algorithm and its variants, as well as version 5.3 of MINOS.

"Starting and Restarting the Primal-Dual Interior POint Method"

We first consider the problem of choosing a starting point for an interior point algorithm for linear programming when no starting point is given. It is shown that incorporation of bounds and reflection of negative values in an analytic formula for estimating the starting point can improve performance over earlier methods. We than consider the problem of restarting the algorithm from a prior optimal solution in order to solve a perturbed problem. We illustrate how the previously optimal solution must be perturbed in order to be able to make adequate progress toward a new optimal point. Preliminary numerical results indicate that convergence to a new optimum is much faster from the perturbed previous optimum than from a cold start.

"An Interior Point Method for Quadratic Programs Based on Conjugate Projected Gradients"

We propose an interior point method for large-scale convex quadratic programming where no assumptions are made about the sparsity structure of the quadratic coefficient matrix Q. The interior point method we describe is a doubly iterative algorithm that invokes a conjugate projected gradient procedure to obtain the search direction. The effect is that Q appears in a direction routine conjugate rather than in a matrix factorization. By doing this, the matrices to be factored have the same nonzero structure as those in linear programming. Further, one variant of this method is theoretically convergent with only one matrix factorization throughout the procedure.