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Final Technical Report

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Research Title : Numerical Methods for Linear and Nonlinear Optimization

Dates: 7/1/86 - 6/30/87

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Summary

Three major objectives were completed during the year. The first demonstrates how to directly use rank-one updates to a Cholesky factorization of the required inverse for Karmarkar projections while fully exploiting sparsity. This can significantly improve computational speed when only a few variables are changing significantly at each step. The second demonstrates a new method for adding new variables to a quasi-Newton Hessian approximation which preserves problem scale and positive definiteness of the Hessian. Numerical results show the method to be preferable to known methods. The third examines a variety of ways of implementing a sequential quadratic programming code, and uses numerical testing to indicate a suitable merit function and good algorithms for updating Lagrange multiplier and Hessian approximations. Recent new results for updating Hessians for unconstrained problems are currently being studied to determine if better Hessian approximations can be obtained. For

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The proposed research was to investigate numerical methods for two constrained optimization problems, linear programming problems and nonlinear programming problems with either linear or nonlinear equality constraints. This report will deal with progress to date and remaining problems of interest for each of these in turn.

The general nonlinear programming problem is

minimize f(x)subject to $g_i(x) = 0, i = 1, ..., m$ and $g_j(x) \le 0, j = m+1, ..., p$.

Here $x = (x_1, \ldots, x_n)^T$, and f(x) is assumed to be nonlinear in at least a subset of the variables. When the constraints are linear, it is well known that this problem can be transformed to the form

> minimize f(x) subject to Ax=b, l≤x≤u,

where 1 and u are vectors of (possibly infinite) upper and lower bounds. Reduced gradient methods fix some of the variables at their bounds, and solve the reduced problem in the remaining free variables. The fixed variables are then tested to ascertain whether a better solution can be found if the variable is allowed to vary freely between its bounds. When a variable is freed, computation of a search direction requires that either the mixed second partial derivatives of f(x) with respect to the variable are explicitly calculated, or if a quasi-Newton approximation to the Hessian is being used, that they be estimated in a way consistent with problem scaling and maintaining positive definiteness of the approximate Hessian. Finite differencing will produce an approximation which is appropriately scaled, but the approximate Hessian need not be positive definite. Adding a row and column with a positive diagonal and zeroes elsewhere will produce a positive definite Hessian, but it is generally poorly scaled.

This research has devised a new method, identical in the amount of work to finite differencing, but which uses the structure of quasi-Newton methods to assure both positive definiteness and proper scaling. The method has been tested numerically, and in limited testing has proved far superior to current alternative methods. It has been documented in the report "Adding Variables to Quasi-Newton Hessian Approximations", which will appear in the <u>Journal of</u> <u>Optimization Theory and Applications</u> in August, 1987.

When the constraints are nonlinear, transformation to slacked equality constraints may or may not cause numerical problems with singular Hessian matrices. When only the Hessian of f(x) is considered, clearly it is singular if slack variables are included in the constraints. If, however, the Hessian is the Hessian of the Lagrangian function, then singularity may not occur. While the problem of transforming inequality to equality constraints for general nonlinear programming is still the subject of a

great deal of research, enough problems can be formulated with strict equality constraints to generate substantial interest in solving the problem

> minimize f(x)subject to $g_i(x) = 0$, i=1,...,m.

The Langrangian of this problem is

$$L(x,) = f(x) - \sum_{i=1}^{m} \lambda_{i} g_{i}(x),$$

and the currently most successful methods for solving the problem are the sequential quadratic programming methods, which attempt to solve the problem by computing the first order conditions for a solution by differentiating the Lagrangian, and then applying Newton's method to solve these first order conditions. Here the search directions can be shown to solve

minimize s^TBs+s^T∇f

subject to $g+N^{T}s=0$,

where N is the matrix of constraint gradients, ∇f the gradient of the objective function, $g=(g_1,\ldots,g_m)^T$, and B is an approximation to the Hessian of the Lagrangian.

As B is an estimate to the Hessian of the Lagrangian, calculation of B requires estimates to the Lagrange multipliers. Further, a sufficient step along s to assure a quasi-Newton approximation to B is positive definite can not always be taken, for the new point may prove to be too far outside the feasible region. Finally, some measure, called a merit function, must be introduced to assure that feasibility and function reduction are kept in reasonable balance.

The goal of this research was to attempt to test various means of estimating λ and B, and to use several different merit functions in an attempt to determine what combination was likely to produce an efficient numerical algorithm. The results of this study have been documented in the report "Numerical Experience wiht Sequential Quadratic Programming", which is under review for the <u>Transactions on Mathematical Software</u> in revised form, having been revised to address the comments of the generally favorable referees. The report addresses the questions raised above in detail, with specific recommendations on merit functions, update strategy, and Lagrange multiplier estimates.

Finally, research is being concluded on more efficient hybrid schemes for updating a Hessian approximations, and will be documented in a report to be submitted to the <u>SIAM</u> Journal on Numerical Analysis.

Recent research in linear programming has been concerned with interior point methods, or methods which follow a trajectory across the interior of the feasible region rather than moving from vertex to vertex. This was initiated by Karmarkar, who used projective transformations to recenter the current estimate at every point, then move toward the boundary.

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The major numerical work in Karmarkar's algorithm is in computing a projection of the form

 $s = (I-DA^{T}(AD^{2}A^{T})^{-1}AD)c,$

where D is a diagonal matrix which changes at each iteration, while A is a fixed matrix. Karmarkar suggests updating a factorization of (AD^2A^T) only for those elements of D which have changed significantly, and shows that this reduces the theoretical complexity of the algorithm.

The report "Computing Karmarkar Projections Quickly", has been accepted for publication in <u>Mathematical</u> <u>Programming</u>. It shows how to update a Cholesky factorization to AD^2A^T in a way that fully and naturally exploits sparsity, and shows that the method has great promise for reducing computation time.

Finally, significant research is continuing on interior point methods. A code implemeting a full primal-dual method is under development, with very promising preliminary results. This is being continued under grant AFSOR-87-0215 to Rutgers University. Articles Accepted, Submitted, and Planned

- 1) D. F. Shanno and K. H. Phua, "Adding Variables to Quasi-Newton Approximations", <u>Journal of Optimization</u> <u>Theory and Application</u> (in press).
- 2) D. F. Shanno and K. H. Phua, "Numerical Experience with Sequential Quadratic Programming Algorithms for Equaltity Constrained Nonlinear Programming", <u>Transactions on</u> <u>Mathematical Software</u> (under review).
- 3) D. F. Shanno, "Computing Karmarkar Projections Quickly", <u>Mathematical Programming</u> (in press).
- 4) D. F. Shanno, "Improved Quasi-Newton Approximations", (in preparation).

Paper presented at meetings

Computing Karmarkar Projections Quickly at the SIAM National Meeting, Boston, MA., July, 1986 and at the ORSA/TIMS Meeting, Miami, October, 1986 (both invited).

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