RESEARCH ON OPTIMIZATION ALGORITHMS AND APPLICATIONS

Progress Report

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Research on Optimization Algorithms and Applications

Annual Progress Report

Abstract

The project had a productive first year with five technical reports produced or in preparation. The major works accomplished include the following: (1) we have conducted investigations on algorithms for global optimization of zero-to-small residual least squares problems. Numerical results have demonstrated the effectiveness of our algorithms on many test problems; (2) we have investigated a fundamental question concerning the behavior of Newton's method on equivalent systems. This investigation will provide guidance to the proper choice of formulations in solving some optimization problems; (3) we have developed and tested new and promising interior-point algorithms for the maximum-volume ellipsoid problem.

1 Main Results

An important activity in X-ray crystallography is to develop effective globalization strategies for solving the semi-local and global stage of the phase problem. The phase problem is posed as a global minimization problem whose objective function is described in a least-squares format. The main objective for the research reported in Technical Report [1] is to investigate some novel techniques for solving such problem at the semi-local stage and make comparisons to available methods and software on the market. In Technical Report [1], we report encouraging initial progress on developing efficient semi-local algorithms for global least-squares data-fitting problems. We have derived a modified Gauss-Newton type method as a global optimization method. For zero or very small residual problems, the iterates generated by this method are attracted to the global minimum, but repelled from local minima of higher residual values. We have tested this approach on some test problems in the literature with success. Combining this approach with a simple multi-start strategy, we have been able to solve small instances of the phase problem in X-ray crystallography from completely random guesses. For

larger problems, we have demonstrated through numerical experiments that our method possesses a larger region of attraction around the global minimizer than does a Gauss-Newton-type method implemented in a widely used software package.

Newton-type methods are fundamental techniques for solving systems of nonlinear equations. However, it is often not fully appreciated that these methods can produce significantly different behavior when applied to equivalent systems. In Technical Report [2], we investigate differences in local and global behavior of Newton-type methods when applied to the first-order optimality conditions for the logarithmic barrier formulation of the linear programming problem, and when applied to the equivalent perturbed first-order optimality conditions for the linear programming problem. Through theoretical analysis and numerical results, we show that Newton-type methods perform more effectively on the latter system than on the former system.

The central theme of Technical Report [3] is the same as that of Technical Report [2], though the two equivalent systems investigated in Technical Report [4] are derived from nonlinear optimization problems with simple bounds.

Research reported in Technical Report [4] is concerned with the problem of finding the maximum-volume ellipsoid contained in a polytope in $\mathbb{R}^n$. This is a fundamental subproblem widely used in the construction of many optimization algorithms. Though a number of theoretical, polynomial algorithms have been proposed for this problem, it is yet not clear that they are practically effective. In Technical Report [4], we propose several interior-point algorithmic formulations for the maximum-volume ellipsoid problem and report preliminary computational results on some of them that we consider to be practically efficient.

Technical Report [5] was finished during the first year of the present project which consists of results obtained during the previous project of the PI, also supported by DOE.

2 Compliance with Requirements

In the first year of the project, we fully complied with the agreement requirements for this grant. During the academic year, the PI devoted to the project a percentage of time exceeding 10%, and in the summer he devoted two months to the project. The research

assistant also fulfilled the agreement requirements. In the second year, we expect that same amount of time and effort, if not more, will be devoted to the project.

3 Technical Reports

We list the technical reports authored or co-authored by the PI during the first year of the project.

- [1] G. Phillips, R. Tapia, L. Velazquez and Y. Zhang. On Global Optimization Techniques with Application to the Least Squares Phase Problem in X-Ray Crystallography. Technical Report TR98-13, Department of Computational and Applied Mathematics, Rice University, Houston, TX 77005. 1998.
- [2] Cristina Villalobos, Richard Tapia and Yin Zhang. The Behavior of Newton-type Methods on Two Equivalent Systems from Linear Programming. Technical Report TR98-02, Department of Computational and Applied Mathematics, Rice University, Houston, TX 77005. 1998.
- [3] Diane Jamrog, Richard Tapia and Yin Zhang. Comparison of Coleman-Li and Perturbed KKT formulations for nonlinear optimization with simple bounds. Technical Report (in preparation), Department of Computational and Applied Mathematics, Rice University, Houston, TX 77005. 1998.
- [4] Yin Zhang. On practical interior-point algorithms for the maximum-volume ellipsoid problem. Technical Report TR98-15, Department of Computational and Applied Mathematics, Rice University, Houston, TX 77005. 1998.
- [5] D. Zhang and Y. Zhang. On Constructing Interior-Point Path-Following Methods for Certain Semimonotone Linear Complementarity Problems. Technical Report TR97-19, Department of Computational and Applied Mathematics, Rice University, Houston, TX 77005. 1997.