Large Scale Computational Problems in Numerical Optimization

Grant: DE-FGO2-86ER25013, Final Report: 1986-2000

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This research effort resulted in 50 research publications, 4 related published books, 10 PhD students produced, and 13 postdoctoral researchers supported (one of whom, Yuying Li, won the 6th FOX prize competition).

Our work under this support broadly falls into five categories: automatic differentiation, sparsity, constraints, parallel computation, and applications.

Automatic Differentiation (AD): We developed strong practical methods for computing sparse Jacobian and Hessian matrices which arise frequently in large scale optimization problems [10,35]. In addition, we developed a novel view of "structure " in applied problems along with AD techniques that allowed for the efficient application of sparse AD techniques to dense, but structured, problems [4,5,9,37,40,41]. Our AD work included development of freely available MATLAB AD software [5].

Sparsity: We developed new effective and practical techniques for exploiting sparsity when solving a variety of optimization problems. These problems include: bound constrained problems, robust regression problems, the null space problem, and sparse orthogonal factorization[8,13,16,18,21,22,28,29,32,33,34,35,38,39,42,47,48]. Our sparsity work included development of freely available and published software [38,39].

Constraints: Effectively handling constraints in large scale optimization remains a challenge. We developed a number of new approaches to constrained problems [2,3,6,7,12,24,26,36] with emphasis on trust region methodologies.

Parallel Computation: Our work included the development of specifically parallel techniques for the linear algebra tasks underpinning optimization algorithms. Our work contributed to the nonlinear least-squares problem, nonlinear equations, triangular systems, orthogonalization, and linear programming [23,25,27,30,38,39,45,49,50].

Applications: Our optimization work is broadly applicable across numerous application domains. Nevertheless we have specifically worked in several application areas including molecular conformation, molecular energy minimization, computational finance, and bone remodeling [1,11,14,15,17,19,20].

We conclude by mentioning that our PhD students have gone to major industry and government labs (such as Sandia), as well as major universities (such as Purdue), and the mathematical software industry more broadly (such as Mathworks, Bloomberg).

Research Refereed Journal Publications under this support

1. Reconstructing the unknown local volatility function, *Journal of Computational Finance*, Vol. 2, No. 3 (Spring,1999), pp. 77—102 (with Yuying Li, Arun Verma).

2. A trust region and affine scaling interior point method for nonconvex minimization with linear inequality constraints, *Mathematical Programming Series A*, 88 (1), pp. 1-32, June 2000 (with Yuying Li).

3. A quasi-Newton quadratic penalty method for minimization subject to nonlinear equality constraints, *Computational Optimization and Applications*, 15, pp. 103-124, Feb. 2000. (with Jianguo Liu & Wei Yuan).

4. Efficient calculation of Jacobian and adjoint vector products in wave propagational inverse problems using automatic differentiation, Journal of Computational Physics 157, pp. 234-255, 2000. (with Fadil Santosa and Arun Verma).

5. ADMIT-1: Automatic differentiation and MATLAB interface toolbox, ACM Transactions on Mathematical Software 22, pp. 150-175 (2000) (with Arun Verma).

6. An exterior Newton method for strictly convex quadratic programming, *Computational Optimization and Applications 15, (2000), pp. 5-32.* (with Jianguo Liu).

7. An interior Newton method for quadratic programming, *Mathematical Programming ,Series A, 85, pp 491-523 (1999).* (with Jianguo Liu).

8. A subspace, interior, and conjugate gradient method for large-scale bound-constrained minimization problems, *SIAM Journal on Scientific Computing 21 (1999), pp. 1-23.* (with M.A. Branch, Yuying Li).

9. The efficient computation of structured gradients using automatic differentiation, *SIAM Journal on Scientific Computing 20*, (1999), pp. 1430-1437 (with Gudbjorn Jonsson).

10. The efficient computation of sparse Jacobian matrices using automatic differentiation, *SIAM Journal on Scientific Computing* 19, (1998) pp. 1210-1233 (with Arun Verma).

11. Parallel continuation-based global optimization for molecular conformation and protein folding, *Journal of Global Optimization* 8, (1996) pp. 49-65. (with Zhijun Wu).

12. An interior trust region approach for nonlinear minimization subject to bounds, *SIAM Journal on Optimization* 6 (1996) pp. 418-445 (with Yuying Li).

13. A reflective Newton method for minimizing a quadratic function subject to bounds on the variables, *SIAM Journal on Optimization* 6 (1996) pp. 1040-1058 (with Yuying Li).

14. An efficient trust region method for unconstrained discrete-time optimal control problems, *Computational Optimization and Applications* 4 (1995) pp. 47-66. (with Ai-ping Liao).

15. Parallel structural optimization applied to bone remodeling on distributed memory machines, *Computational Optimization and Applications* 4 (1995) pp. 375-392. (with Shirish Chinchalkar).

16. On the convergence of reflective Newton methods for large-scale nonlinear minimization subject to bounds, *Mathematical Programming* 67, Series A (1994) pp. 189-224. (with Yuying Li).

17. A parallel build-up algorithm for global energy minimizations of molecular clusters using effective energy simulated annealing, *Journal of Global Optimization* 4 (1994) pp. 171-185. (with Zhijun Wu).

18. A globally and superlinearly convergent algorithm for convex quadratic programs with simple bounds, *SIAM Journal on Optimization* 3 (1993) pp. 298 - 321 (with L. Hulbert).

19. Isotropic effective energy simulated annealing searches for low energy molecular cluster states, *Computational Optimization and Applications* 2 (1993) pp. 145 - 170, (with David Shalloway, Zhijun Wu).

20. Parallel finite element analysis of biomechanical structures on the Ncube 6400, *Mathematical Modelling and Scientific Computing* 1, (1993) pp 126-141 (with Shirish Chinchalkar).

21. A globally and quadratically convergent affine scaling method for linear l_1 problems, *Mathematical Programmin*g 56, Series A, (1992) pp. 189-222 (with Yuying Li).

22. A global and quadratically convergent method for linear l_∞ problems, *SIAM Journal on Numerical Analysis* 29, (1992) pp. 1166-1186 (with Yuying Li).

23. A parallel nonlinear least-squares solver: theoretical analysis and numerical results. *SIAM Journal on Scientific and Statistical Computing* 13, (1992) 771-793 (with P. Plassmann).

24. Partitioned quasi-Newton methods for nonlinear equality constrained optimization, *Mathematical Programming* 53 (1992) 17-44 (with P. Fenyes).

25. Solving systems of nonlinear equations on a message-passing multiprocessor, *SIAM Journal on Scientific and Statistical Computing* 11, (1990) 1116-1135 (with Guangye Li).

26. Computing a trust region step for a penalty function, *SIAM Journal on Scientific and Statistical Computing* 11, (1990) 180-201 (with C. Hempel).

27. A new method for solving triangular systems on distributed memory message-passing multiprocessors *SIAM Journal on Scientific and Statistical Computing* 10, (1989) 382-396 (with Guangye Li).

28. A direct active set algorithm for large sparse quadratic programs with simple bounds, *Mathematical Programming*, Series B, 45(1989) 373-406, (with L. Hulbert).

29. Chordal preconditioners for large scale optimization, *Mathematical Programming* 40, (1988) 265-287.

30. A parallel triangular solver for a distributed memory multiprocessor, *SIAM Journal on Scientific and Statistical Computing* 9, (1988) 485-502 (with Guangye Li).

31. Local convergence of the multi-secant method for the parallel solution of systems of nonlinear equations, *Applied Mathematics Letters* 1, (1988) pp. 141-146 (with Guangye Li).

32. The null space problem II. algorithms. *SIAM Journal on Algebraic and Discrete Methods* 8, (1987), 544-563 (with A. Pothen).

33. Predicting fill for sparse orthogonal factorization. *Journal of the Association for Computing Machinery* 83, (1986) 517-532 (with J. Gilbert, A. Edenbrandt).

34. The null space problem I. complexity. *SIAM Journal on Algebraic and Discrete Methods* 7, (1986) 527-539 (with A. Pothen).

35. The cyclic coloring problem and estimation of sparse Hessian matrices. *SIAM Journal on Algebraic and Discrete Methods* 7, (1986) 221-235 (with J. Cai).

Other Published Research Publications under this support

36. Combining trust region and affine scaling for linearly constrained nonconvex minimization, in *Advances in Nonlinear Programming, Proceedings of the 1996 International Conference on Nonlinear Programming*, Ya-Xiang Yuan editor, pp. 219-250, Kluwer Academic Publishers, 1998.

37. Structure and efficient Hessian calculation, in *Advances in Nonlinear Programming, Proceedings of the 1996 International Conference on Nonlinear Programming*, Ya-Xiang Yuan editor, pp. 57-72, Kluwer Academic Publishers, 1998.

38. pPCx: Solving linear programs in parallel in *SIAG/OPT Views-and-Ne*ws, Newsletter for SIAM Activity Group on Optimization, No. 9, pp. 1-5, Fall 1997. (with Chunguang Sun, Michael Wagner).

39. pPCx: Parallel software for linear programming, in *Proceedings of the Eighth SIAM Conference on Parallel Processing for Scientific Computing*, Minneapolis, March, 1997. (with Joseph Czyzyk, Chunguang Sun, Michael Wagner, Stephen Wright).

40. Semi-automatic differentiation, in *Computational Methods for Optimal design and Control*, Jeff Borggaard, John Burns, Eugene Cliff, and Scott Schreck (eds), Birkhauser, 1998, pp. 113-126 (with Fadil Santosa and Arun Verma).

41. Structure and efficient Jacobian calculation, in *Computational Differentiation: Techniques, Applications, and Tools*, Martin Berz, Christian Bischof, George Corliss, Andreas Griewank (eds.), SIAM, Philadelphia, Penn., 1996, pp. 149-159. (with Arun Verma).

42. Linearly constrained optimization and projected preconditioned conjugate gradients, in *Proceedings of the Fifth SIAM Conference on Applied Linear Algebra* pp. 118-122, 1994, SIAM Publications.

43. Large-scale numerical optimization: Introduction and overview, in *Encyclopedia of Computer Science and Technology* Volume 28, Supplement 1S, Marcel Dekker, 1993, pp. 167 - 196.

44. On the local convergence of the Byrd-Schnabel algorithm for constrained optimization, *Applied Mathematics Letters* 6, 1993, pp. 37-42, (with Ai-Ping Liao).

45. Parallel orthogonal factorizations of large sparse matrices on distributed-memory multiprocessors, *in Proceedings of the Sixth SIAM Conference on Parallel Processing for Scientific Computing*, Vol. 1, pp. 457-461, 1993, SIAM Publications (with Chunguang Sun).

46. On characterizations of superlinear convergence for constrained optimization, in *Lectures in Applied Mathematics, Volume 26, Computational Solution of Nonlinear Systems of Equations*, pp. 113-134, AMS, 1990.

47. A quadratically-convergent algorithm for the linear programming problem with lower and upper bounds, in *Large-Scale Numerical Optimization*, T. Coleman and Yuying Li, eds., SIAM, pp. 49-57, 1990 (with Yuying Li).

48. A global and quadratic affine scaling method for (augmented) linear l_1 problems, in *Numerical Analysis* 1989, D.F. Griffiths and G.A. Watson eds., Longman Scientific & Technical, pp. 60-73, 1990 (with Yuying Li).

49. Solution of nonlinear least-square problems on a multiprocessor, in *Parallel Computing*, Springer-Verlag, pp. 4~80, 1988 (with P. Plassmann).

50. A parallel triangular solver for a hypercube multiprocessor, in *Hypercube Multiprocessors*, pp. 539-551, SIAM, 1987 (with Guangye Li).

Related Books Published in this Period

1. Optimization Toolbox, Users Guide, Version 2 (with Mary Ann Branch, Andrew Grace), The Mathworks, Inc., 1999.

2. Large-Scale Optimization with Applications, (ed., with L.Biegler, A. Conn, F. Santosa), Volumes I-III, in *The IMA Volumes in Mathematics and its Applications*, Springer-Verlag, 1997

3. Large-Scale Numerical Optimization, (ed., with Yuying Li), SIAM, Philadelphia, (1990).

4. Handbook for Matrix Computations, (with C. Van Loan) SIAM, Philadelphia, (1988).

PhD Students under this support

1. **Adrian Mariano**, *Image Processing with Total Variation Minimization,* Center for Applied Mathematics (May, 1999)

2. **Arun Verma**, *Structured Automatic Differentiation,* Computer Science Department (May 1998).

3. **Mary Ann Branch**, *An Inexact Reflective Newton Method for Large-Scale Bound Constrained Minimization,* Computer Science Department (August 1995).

4. **Wei Yuan**, *Nonlinear Equality Constrained Minimization via The Quadratic Loss Penalty Function*, Center for Applied Mathematics (August 1995).

5. **Jianguo Liu**, *Interior and Exterior Methods for Large-Scale Quadratic Programming*, Center for Applied Mathematics (August 1994).

6. **Bruce Hendrickson**, *The Molecule Problem: Determining Conformation From Pairwise Distances*, Computer Science Department (January 1991).

7. **Laurie Hulbert,** *Solving Large Sparse Quadratic Programs with Simple Bounds*, Center for Applied Mathematics (April 1990).

8. **Paul Plassmann**, *Parallel Methods for Nonlinear Least Squares Problems*, Center for Applied Mathematics (January 1990).

9. **Chris Hempel,** *Trust Region Methods for the Quadratic Loss Penalty Function,* Center for Applied Mathematics (August 1989).

10. **Peter Fenyes**, *Partitioned Quasi-Newton Methods For Equality Constrained Optimization,* Mechanical and Aerospace Engineering (February 1987).

Postdoctoral Researchers (partially) supported under this grant

1. **Jacqueline Huang** (Johns Hopkins), 1999 – 200

2. **Arun Verma** (Cornell,CS), 1998 -- 2000
3. **Jean-François Pusztaszeri** (CERN, Switzerland) , 1997 -- 1998
4. **Chris Wohlever** (Cornell, TAM), 1996 -- 1997
5. **Ai-ping Liao** (Cornell, ORIE) , 1992 -- 1995
6. **Chunguang Sun** (Penn State), 1991 -- 1994
7. **Li-zhi Liao** (Cornell, ORIE), 1992 -- 1994
8. **Shirish Chinchalkar** (Cornell, MAE), 1991 -- 1993
9. **Zhijun Wu** (Rice), 1991 -- 1993
10. **Danny Ralph** (U. Wisconsin), 1990 -- 1992
11. **Yuying Li** (U. Waterloo), 1988 – 1990, Winner of the 6th FOX Prize competition, Oxford.
12. **Pierre De Mazancourt** (Stanford), 1998 – 1990
13. **Guangye Li** (Rice), 1986 -- 1988

Solving large numerical optimization problems in HPC with python. Antonio GÃ³mez-Iglesias. PyHPC 2015. 1. CONCLUSIONS. â–¶ Python is great for optimization of large-scale problems in HPC resources.Â â–¶ Large number of parameters â–¶ Long wall time â–¶ High computational requirements â–¶ Advancements in software and hardware allow to solve problems that were unfeasible â–¶ Applications on science, society and industry â–¶ Few people working on this, high demand of skills and knowledge. Antonio GÃ³mez-Iglesias. Optimization with Python. PyHPC 2015. 3. Optimizing plasma confinement. Antonio GÃ³mez-Iglesias. Optimization with Python. PyHPC 2015. 4.