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Project Title: Newton Iterative Methods for Large Scale Nonlinear Systems

Principal Investigator: Homer F. Walker

Co-Principal Investigator: Kathryn Turner

Address: Mathematics and Statistics Department Telephone: (801) 750-2026
Utah State University Electronic mail: walker@math.usu.edu
Logan, UT 84322-3900 FAX: (801) 750-1822

1. Introduction.

Newton iterative methods, also known as truncated Newton methods, are implementations of Newton's method in which an iterative linear solver is used to solve approximately the linear systems that characterize Newton steps. These methods are particularly appropriate for large-scale problems in which iterative linear algebra methods are preferred. They are currently used in many important scientific applications, including many of major industrial importance, e.g., aircraft dynamics modeling at Boeing and semiconductor modeling at Bell Labs. In addition to their effectiveness on important problems, these methods also offer a nonlinear "framework" within which to transfer to the nonlinear setting any advances in linear system solving, such as new iterative methods for nonsymmetric linear systems or algorithms that exploit advanced machine architectures. In spite of their conceptual simplicity, these methods involve complex issues; we note particularly the following:

- How accurate should each approximate Newton step be, i.e., when should the linear iterations be stopped, in order to enhance efficiency and robustness away from a solution and ensure fast convergence near a solution?
- How can a method be "globalized" compatibly with the strategy for stopping the linear iterations and other algorithmic features?
- Which iterative linear solver is best suited for the overall method and perhaps a particular problem or computer architecture as well?

The primary objective of this research is to develop robust and efficient Newton iterative methods for general large scale problems that are especially well suited for discretizations of partial differential equations, integral equations, and other continuous problems. A concomitant objective is to develop improved iterative linear algebra methods; this is natural because of both the central role of iterative linear solvers in Newton iterative methods and the current rapid evolution of iterative linear solvers for nonsymmetric linear systems.

Referencing conventions are as follows: Publications acknowledging support from this grant are referenced by [P...] and listed in §2.4. Supplementary references are referenced by [SR...] and listed in §2.5.

2. Technical progress and activities during the current budget period.

We first outline research on Newton iterative methods and then review work on iterative linear algebra methods.

2.1. Newton iterative methods.

2.1.1. Inexact Newton methods.

General, theoretically sound frameworks for Newton iterative methods have been notably absent from the literature, and a preliminary goal of this research has been to develop such frameworks. An ideal general context for this is that of an inexact Newton method [SR1], in which each step reduces the norm of the local linear model of F . Specifically, at the k th iteration of an inexact Newton method, the step s_k satisfies an *inexact Newton condition* $\|F(x_k) + F'(x_k) s_k\| \leq \eta_k \|F(x_k)\|$ for some $\eta_k \in [0, 1)$. A Newton iterative method is naturally a special case of an inexact Newton method: At the k th step, we first choose η_k and then apply the iterative linear solver to $F'(x_k) s = -F(x_k)$ until the inexact Newton condition holds. Used in this way, the η_k 's are often called *forcing terms*. Note that the issue of when to stop the linear iterations is now the issue of choosing η_k . It is shown in [SR1] that local convergence is controlled by the choices of the η_k 's. However, that paper does not address either global convergence or deeper issues associated with choices of the η_k 's.

In [P2], we have formulated a number of inexact Newton methods with strong global convergence properties. These include a number of methods that are well-suited for practical implementation as Newton iterative methods, as well as several abstract methods that can be used to obtain global convergence results for well-known Newton-like methods such as trust region methods. This paper was first submitted for publication in March, 1991. It underwent two revisions during the current budget period (in August, 1992, and March, 1993) before being accepted for publication in March, 1993.

In follow-up work to [P2], we have addressed the issue of making refined choices of the η_k 's. Choices that have previously been proposed result in fast convergence near a solution but do not adequately address efficiency and robustness away from a solution. The central issue is that of *oversolving* the linear system $F'(x_k) s = -F(x_k)$, i.e., going to the expense of reducing the linear residual norm, which is also the local linear model norm, beyond the point at which the local linear model begins to depart significantly from the nonlinear function. We have now arrived at several very promising choices of the η_k 's that minimize oversolving on a number of realistic test problems while retaining fast convergence near a solution. Furthermore, our testing indicates that, by maintaining good agreement between the nonlinear function and its local linear model, these choices relieve the globalization of much of its burden and consequently enhance the robustness of the method. This work is nearly completed and will be written up in [P3].

2.1.2. A GMRES-backtracking Newton iterative method.

A general inexact Newton backtracking method is formulated in [P2] that has strong global convergence properties and allows for desirable choices of the η_k 's as in [P3] (see above). We have developed a Newton iterative implementation of this method that uses restarted GMRES [SR3] as the iterative linear solver. GMRES is a natural first choice for the iterative linear solver because it is robust, generally applicable, relatively well understood, and has the attractive property of reducing the residual norm monotonically; other solvers will be implemented in future work. In our implementation, the user can elect either analytic or finite-difference evaluations of Jacobian-vector products; if finite differences are used, then accuracy is enhanced with low-cost selective central-differencing as in [SR5]. GMRES iterations are terminated using a particular choice of the η_k 's

found in [P3] to be effective for general use. The user can supply a preconditioner and, if desired, an inner-product to be used in place of the default Euclidean inner-product.

An initial version of this implementation and its performance on a set of test problems (PDE's and integral equations) was described in [SR7]. Development has continued and, at present, this implementation can be considered a high-level experimental code. A major goal of this research is to develop a robust, efficient, flexible, portable Newton iterative code that is suitable for public distribution. We feel that the present code is a significant step toward this goal and will provide an excellent basis for future work.

We have also begun investigating trust region-like augmentations of the backtracking method. In its original form, the method relies entirely on an inexact Newton criterion for terminating the GMRES iterations at each step. In theory, this is sufficient; in practice, however, we have seen that it can lead to destructively long steps when the Jacobian is not well-conditioned. We intend to add procedures that will terminate the GMRES iterations when the length of a step produced by GMRES exceeds a trust region radius. This should significantly improve the robustness of the method on some problems. The cost is likely to be minor in most practical problems: Over m steps, GMRES costs $O(m^2n)$ arithmetic operations plus m matrix-vector products; one can monitor the lengths of these m steps for only $O(m^3)$ additional arithmetic. This work is being done jointly with K. Vang, a Ph.D. student at Utah State working under the direction of one of us (Turner).

2.2. Iterative linear algebra methods.

In recent years, there has been a remarkable proliferation of *Krylov subspace methods* for nonsymmetric linear systems. (See [SR2] and the many references therein for a discussion of general Krylov subspace methods and all of the specific methods referred to in the following.) Among current methods, GMRES is the most widely used and is likely to remain of central importance. However, the increasing cost per iteration of GMRES caused much attention to turn in the late 1980's toward short-recursion Lanczos-based methods such as the biconjugate gradient (BCG) and conjugate-gradient squared (CGS) methods. Although BCG and CGS have had some successes where GMRES has not done well, a major shortcoming of these methods is that the residual norms of the iterates often oscillate wildly, which is at least unattractive and can create serious numerical problems as well. This shortcoming has provided important impetus for the development of various BiCGSTAB- and QMR-type methods in the last few years; these produce residual norm sequences that, although not monotone decreasing, are usually but not always fairly well-behaved.

This proliferation shows no signs of abating, and the current spectrum of methods and method approaches offers both challenges and opportunities. Our work to date has centered around GMRES and "residual smoothing" techniques for general iterative linear solvers.

2.2.1. GMRES work.

Our GMRES work has been directed toward developing more accurate and more efficient implementations. In joint work with L. Zhou [P4], a Ph.D. student at Utah State University under the direction of one of us (Walker), we outlined Gram-Schmidt and Householder implementations of GMRES that are simpler than the usual ones (see [SR3], [SR6]). In these, the GMRES least-squares problem emerges in upper-triangular form rather than upper-Hessenberg form, so no Givens rotations are necessary; in addition, the residual vector is always available at no cost in the Gram-Schmidt implementation.

We have also been working with P. N. Brown in the Computation and Mathematics Research Division (CMRD) at Lawrence Livermore National Laboratory (LLNL) to investigate the performance of GMRES on singular or ill-conditioned systems. This should result in implementations

with improved capabilities for detecting and handling ill-conditioning when it threatens to degrade the performance of the method. This work is almost complete and will be written up in [P1].

2.2.2. Residual smoothing techniques.

In further work with L. Zhou [P5], we have investigated “residual smoothing” techniques for general iterative linear solvers. These produce from a given sequence of iterates $\{x_k\}$ an auxiliary sequence $\{y_k\}$ by $y_0 = x_0$ and $y_k = (1 - \xi_k)y_{k-1} + \xi_k x_k$, $k = 1, 2, \dots$, where the ξ_k ’s are chosen to produce “smoothly decreasing” residual norm sequences. In [P5], we first give a numerically sound formulation of *minimal residual smoothing*, originally introduced by Schönaauer [SR4] and Weiss [SR8], in which the ξ_k ’s are chosen to minimize $\|y_k\|_2$. We then show that, by making certain alternative choices of the ξ_k ’s one can obtain various QMR-type methods as smoothings of more basic methods such as BCG, CGS, and BiCGSTAB. This is then extended to a general *QMR smoothing*, applicable to any method.

These smoothing techniques offer valuable practical tools. Minimal residual smoothing allows the straightforward generation of a sequence with monotone decreasing residual norms from a sequence of iterates produced by *any* method. Monotone decreasing residual norms may be a real advantage or just a nicety, depending on the application. Be that as it may, we have found in experiments that smoothing serves the very important function of stabilizing the iterates and residuals when the limits of residual reduction are reached, even though the original method has lost all accuracy and produces inaccurate residual norms that continue, misleadingly, to decrease.

Furthermore, these techniques give an important new perspective on QMR-type methods. In addition to providing a straightforward means of deriving a QMR-type method from any method, they show that QMR-type methods can be properly regarded as just one class of methods among many that can be obtained by applying residual smoothing to more basic methods such as BCG, CGS, and BiCGSTAB.

2.3. Other activities.

2.3.1. Collaborative and advisory activities.

We have noted collaborations above with P. N. Brown (CMRD, LLNL) and S. Eisenstat (Computer Science, Yale) and work with Utah State graduate students K. Vang and L. Zhou. In addition, one of us (Walker) has worked with A. Skjellum (formerly in the CMRD at LLNL, now at Mississippi State), Brown, and others in the CMRD to develop a number of different GMRES implementations based on previous [SR6] and current [P4] work. These implementations differ in the amount and level of BLAS¹ used in them and consequently have differing potentials for exploiting different vector and parallel architectures. One of them was chosen to be the implementation of GMRES in the *Multicomputer Toolbox*, a parallel computing software toolbox under development by Skjellum and the CMRD group. Fortran versions of all of these implementations have been made publicly available through Netlib.

2.3.2. Invited talks.

Invited talks (by Walker) on research supported by this grant during the current budget period are as follows:

- [T1] *Residual smoothing methods for iterative linear system solvers*, Lawrence Livermore National Laboratory, August, 1992.

¹ Basic Linear Algebra Subroutines; see [LAPACK].

- [T2] *Iterative methods for large scale linear and nonlinear systems*, Frontiers Lectures program (three lectures), Mathematics Department, Texas A&M University, October-November, 1992.
- [T3] *Inexact Newton and Newton iterative methods*, Mathematics Department, University of Houston, November, 1992.
- [T4] *A GMRES-backtracking Newton iterative method*, Special Session on Numerical Optimization, AMS 879th Meeting, Knoxville, Tennessee, March, 1993.
- [T5] *Inexact Newton and Newton iterative methods*, International Meeting on Linear/Nonlinear Iterative Methods and Verification of Solution, Matsuyama, Japan, July, 1993.

2.4. Publications.

Publications supported through this grant and acknowledging its support, including those in preparation, are the following:

- [P1] P. N. Brown and H. F. Walker, *GMRES on (nearly) singular systems*, in preparation.
- [P2] S. C. Eisenstat and H. F. Walker, *Globally convergent inexact Newton methods*, Utah State University Math. Stat. Dept. Res. Report February/91/51, February, 1991 (revised July, 1992 and March, 1993), to appear in SIAM J. Optimization.
- [P3] S. C. Eisenstat and H. F. Walker, *Choosing the forcing terms in an inexact Newton method*, in preparation.
- [P4] H. F. Walker and L. Zhou, *A simpler GMRES*, Utah State University Math. Stat. Dept. Res. Report 1/92/54, January, 1992 (revised October, 1992), to appear in J. Numer. Lin. Alg. Appl.
- [P5] L. Zhou and H. F. Walker, *Residual smoothing techniques for iterative methods*, Utah State University Math. Stat. Dept. Res. Report 5/92/58, May, 1992 (revised December, 1992), to appear in SIAM J. Sci. Comput.

2.5. Supplementary references.

- [SR1] R. Dembo, S. C. Eisenstat, and T. Steihaug, *Inexact Newton methods*, SIAM J. Numer. Anal., 19 (1982), pp. 400–408.
- [SR2] R. W. Freund, G. H. Golub, and N. M. Nachtigal, *Recent advances in Lanczos-based iterative methods for nonsymmetric linear systems*, Acta Numerica 1992, Cambridge University Press, 1992, pp. 57–100.
- [SR3] Y. Saad and M. H. Schultz, *GMRES: a generalized minimal residual method for solving nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 7 (1986), pp. 856–869.
- [SR4] W. Schönauer, *Scientific Computing on Vector Computers*, North-Holland, Amsterdam, 1987.
- [SR5] K. Turner and H. F. Walker, *Efficient high accuracy solutions with GMRES(m)*, SIAM J. Sci. Stat. Comput., 13 (1992), pp. 815–825.
- [SR6] H. F. Walker, *Implementations of the GMRES method*, Computer Physics Communications, 53 (1989), pp. 311–320.
- [SR7] H. F. Walker, *A GMRES-backtracking Newton iterative method*, Proceedings of the Conference on Iterative Methods, Copper Mountain, Colorado, April, 1992.
- [SR8] R. Weiss, *Convergence Behavior of Generalized Conjugate Gradient Methods*, Ph.D. dissertation, University of Karlsruhe, 1990.

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