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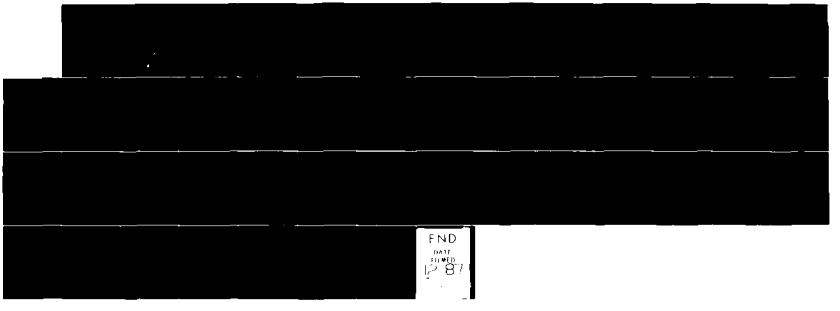

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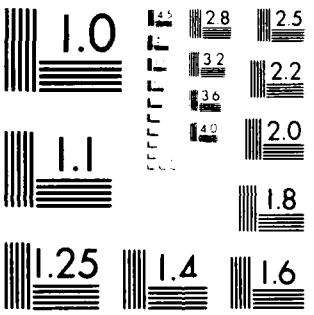

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Computational Behavior of Gauss-Newton Methods

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Computational Behavior of Gauss-Newton Methods

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Abstract

This paper is concerned with the numerical behavior of Gauss-Newton methods for nonlinear least-squares problems. Here we assume that the defining feature of a Gauss-Newton method is that the direction from one iterate to the next is the numerical solution of a particular linear least-squares problem, with a steplength subsequently determined by a linesearch procedure. It is well known that Gauss-Newton methods cannot be successfully applied to nonlinear least-squares problems as a class without modification. Our purpose is to give specific examples illustrating some of the difficulties that arise in practice which we believe have not been fully described in the literature.

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1. Introduction

The nonlinear least-squares problem is given by

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \sum_{i=1}^{m} \phi_i^2(x),$$

where $\phi_i(x)$ are real-valued functions, or, equivalently,

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \|f(x)\|_2^2,$$

where

$$f(x) = \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \\ \vdots \\ \phi_m(x) \end{pmatrix}.$$

We assume that each ϕ_i has continuous second partial derivatives. The function $\frac{1}{2} \|f(x)\|_2^2$ will be called the *least-squares objective function.*

The classical approach to nonlinear least squares, called the *Gauss-Newton* method, locally approximates each residual component ϕ_i of f by a linear function, using the relationship

$$f(x+p) \approx f(x) + J(x)p + \mathcal{O}(\|p\|^2), \tag{1.1}$$

where J is the Jacobian matrix of f, that is

$$J(x) \equiv \nabla f(x) = \begin{pmatrix} \frac{\partial \phi_1}{\partial x_1} & \cdots & \frac{\partial \phi_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial \phi_m}{\partial x_1} & \cdots & \frac{\partial \phi_m}{\partial x_n} \end{pmatrix}.$$

The step to the new iterate from the current point is in the direction of the vector p that solves

$$\min_{p \in \mathbb{R}^n} \|f + Jp\|_2^2;$$

in other words, the change in the nonlinear least-squares objective $\frac{1}{2} f^T f$ is being modeled by the quadratic function

$$\bar{g}^T p + \frac{1}{2} p^T J^T J p,$$

where

$$\bar{g} \equiv \nabla \left(\frac{1}{2} f^T f \right) = J^T f. \tag{1.2}$$

Hence the Gauss-Newton method differs from Newton's method in that the Hessian matrix

$$\nabla^2 \left(\frac{1}{2} f^T f \right) = J^T J + \sum_{i=1}^{m} \phi_i \nabla^2 \phi_i$$

is approximated by $J^T J$, a strategy that would seem reasonable when the residuals are small.

Although it is well known that the Gauss-Newton method does not work well under all circumstances, it is not possible to say anything more precise about the method when considering large and varied sets of test problems. Detailed numerical study is essential in order to understand the practical shortcomings of the Gauss-Newton method. In this paper we analyze specific examples of performance that reveal some of the difficulties that may be encountered in practice.

1.1. Overview

In Section 2, we show that a class of numerical methods, rather than a single method, is defined by the linearization (1.1) of f, and motivate these methods from considerations that arise in unconstrained optimization (see, for example, Fletcher [1980], Gill, Murray, and Wright [1981], Dennis and Schnabel [1983], or Moré and Sorensen [1984]) and linear least squares (see, for example, Stewart [1973], Lawson and Hanson [1974], or Golub and Van Loan [1983]). Section 3 surveys research related to computational aspects of Gauss-Newton methods. In Section 4, we give a general description of how the numerical results presented in the remaining sections of the paper were obtained. Examples of the performance of Gauss-Newton methods on problems with ill-conditioned Jacobians are presented in Section 5. An example of poor performance of a Gauss-Newton method on a zero-residual problem with a well-conditioned Jacobian is analyzed in Section 6. Tables of numerical results for two different Gauss-Newton methods for a large set of test problems are included in an appendix.

1.2. Notation

Generally subscripts on a function mean that the function is evaluated at the corresponding subscripted variable (for example, $f_k = f(x_k)$). An exception is made for the residual functions ϕ_i, where the subscript is the component index within the vector f.

2. Motivation

The Gauss-Newton method for nonlinear least squares can be viewed as a modification of Newton's method in which $J^T J$ is used to approximate the Hessian matrix of the least-squares objective function

$$J(x)^T J(x) + \sum_{i=1}^{m} \phi_i(x) \nabla^2 \phi_i(x).$$

Two promising aspects of this approximation are that computation of $J^T J$ involves only first derivatives, and that $J^T J$ is always at least positive semi-definite. Moreover, if $f(x^*) = 0$ and $J(x^*)^T J(x^*)$ is positive-definite, then x^* is an isolated local minimum and the method is locally quadratically convergent. To see this, define

$$B \equiv \sum_{i=1}^{m} \phi_i(x) \nabla^2 \phi_i(x),$$

(B is the neglected term in the Hessian) and consider the expansion of (1.2):

$$0 = J(x^*)^T f(x^*) = \bar{g} + \left(J^T J + B\right)(x - x^*) + \mathcal{O}(\|x - x^*\|^2),$$

which is valid since it is assumed that f has continuous second derivatives. The Gauss-Newton search direction at the current iterate minimizes the quadratic function

$$\bar{g}^T p + \frac{1}{2} p^T J^T J p, \tag{2.1}$$

and therefore satisfies the equations

$$J^T J p = -\bar{g}. \tag{2.2}$$

Because $J(x^*)^T J(x^*)$ is positive definite and J is continuous, $\left(J^T J\right)^{-1}$ exists and has bounded norm in a neighborhood of x^*. Hence convergence is quadratic when $\left\|\left(J^T J\right)^{-1} B\right\|$ is $\mathcal{O}(\|x - x^*\|)$. In particular, quadratic convergence must eventually occur whenever $f(x^*) = 0$, because then $\|f\|$ is $\mathcal{O}(\|x - x^*\|)$ (and so is $\|B\|$). When the objective vanishes at a minimum, (2.1) is an $\mathcal{O}\|p\|^2$ approximation to $\frac{1}{2}\left(\|f(x+p)\|_2^2 - \|f(x)\|_2^2\right)$, so that in the limit the Gauss-Newton direction approaches the Newton search direction p_N, which satisfies

$$\left(J^T J + B\right) p_N = -\bar{g}.$$

When $f(x^*) \neq 0$, the Gauss-Newton method will converge linearly if the smallest singular value of $J^T J$ exceeds the largest singular value of B, but may otherwise diverge. It is not convergent

when the minimum singular value of B exceeds the maximum singular value of J^TJ in a neighborhood of a solution. For more detailed convergence analysis see, for example, Osborne [1972], McKeown [1975a, 1975b], Ramsin and Wedin [1977], Deuflhard and Apostolescu [1980], Dennis and Schnabel [1983, Chapter 10], Schaback [1985], and Häussler [1986].

A drawback of the Gauss-Newton method is that when J^TJ is singular, or, equivalently, when J has linearly dependent columns, (2.1) does not have a unique minimizer. For this reason the Gauss-Newton method should more accurately be viewed as a class of methods, each member being distinguished by a different choice of p when J^TJ is singular. The set of vectors that minimize (2.1) is the same as the set of solutions to the linear least-squares problem

$$\min_{p\in\mathbb{R}^n} \|Jp + f\|_2 . \tag{2.3}$$

One (theoretically) well-defined alternative that is often approximated computationally is to require the unique solution of minimum l_2 norm:

$$\min_{p\in S} \|p\|_2 , \tag{2.4}$$

where S is the set of solutions to (2.3), while another is to replace J in (2.3) by a maximal linearly independent subset of its columns (see, for example, the references cited above on linear least squares). In finite-precision arithmetic, there is often some ambiguity about how to formulate and solve these alternative subproblems when the columns of J are "nearly" linearly dependent, so that, from a computational standpoint, any particular Gauss-Newton method must be still viewed as a class of methods. The references cited above for linear least squares discuss at length the difficulties inherent in computing solutions to (2.3) when J is ill-conditioned, and show that the numerical solution of these problems is dependent on the criteria used to estimate the rank of J. From now on, the term "Gauss-Newton method" will refer to any linesearch method in which the search direction is the result of any well-defined computational procedure for solving (2.3).

For the moment, assume that a solution p to (2.3) can be computed. Then because p satisfies (2.2), p is a direction of descent for f^Tf whenever $J^Tf \neq 0$ (in other words, $\bar{g}^Tp < 0$, so that f^Tf initially decreases along p). To guarantee convergence, the search direction must also be bounded away from orthogonality to the gradient, a condition that may not be met by a Gauss-Newton method unless the eigenvalues of J^TJ are bounded away from zero for the sequence of iterates. Powell [1970] gives an example of convergence of a Gauss-Newton method

with exact line search to a non-stationary point. Moreover, when $J^T J$ is nearly singular, the (unique) solution to (2.2) can be very large in magnitude compared to $\|J\|_2$ and $\|f\|_2$.

Bounding the norm of the solution is a major concern in formulating criteria for rank estimation and solution of linear least-squares problems in finite-precision arithmetic, largely because numerical solutions to (2.3) may not be very accurate when the columns of J are nearly linearly dependent (see the references cited above on linear least squares). In the context of nonlinear least squares, another reason to avoid large search directions is that numerical linesearch methods may not be able to determine an adequate step length when $\|p\|_2$ is large. Moreover, the angle between p and $\bar{g}$ may be taken into account in estimating the rank of J, since p must be a descent direction for $f^T f$ that is bounded away from orthogonality to the gradient. We shall see in Section 5 that, even with these additional considerations that can be brought to bear on (2.3) due to the outer linesearch algorithm, it may be very difficult to give a numerical definition of rank.

The performance of Gauss-Newton methods is not fully understood. Gauss-Newton methods are of practical interest because there are many instances in which they work very well in comparison to other methods, and in fact most successful specialized approaches to nonlinear least-squares problems are based to some extent on Gauss-Newton methods and attempt to exploit this behavior whenever possible (for a survey, see Fraley [1987]). However, it is not hard to find cases where Gauss-Newton methods perform poorly, so that they cannot be successfully applied without modification to general nonlinear least-squares problems. These remarks will be substantiated by examples in Sections 5 and 6.

Perhaps a reason for the variability in the performance of Gauss-Newton methods is that they are not theoretically well-defined. To see this, let $Q(x)$ be a $k \times m$ orthogonal matrix function on $\Re^n$, that is, $Q(x)^T Q(x) = I$ for all x. Then $\|Q(x)f(x)\|_2^2 = \|f(x)\|_2^2$ for all x, and consequently the function $\tilde{f} \equiv Qf$ defines the same nonlinear least-squares problem as f. The Jacobian matrix of $\tilde{f}$ is $\tilde{J} \equiv QJ + (\nabla Q)f$, so that a minimizer of $\|\tilde{J}p + \tilde{f}\|_2$ will ordinarily be different from a minimizer of $\|Jp + f\|_2$, unless $Q(x)$ happens to be a constant transformation. However, if both Q and f have k continuous derivatives, then $\nabla^i \|Q(x)f(x)\|_2^2 = \nabla^i \|f(x)\|_2^2$ for $i = 1, 2, \ldots, k$. Letting $W \equiv (\nabla Q)f$, so that $\tilde{J} = QJ + W$, we have

$$\tilde{J}^T \tilde{J} = J^T J + (J^T Q^T W + W^T Q J) + W^T W,$$

showing that the Gauss-Newton approximation $J^T J$ to the full Hessian matrix is changed when f is transformed by an orthogonal function that varies with x. Thus, with exact arithmetic, there are many Gauss-Newton methods corresponding to a given vector function (in fact, each step of a Gauss-Newton method could be defined by a different transformation of f), although Newton's method remains invariant (see also Nocedal and Overton [1985], p. 826). Moreover, the conditioning of $\tilde{J}$ may be very different from that of J, so that, for example, the columns of $\tilde{J}$ might be strongly independent, while J is nearly rank deficient. Since k may be greater than n, it is possible to imbed the given nonlinear least-squares problem in a larger one. To the best of our knowledge the idea of preconditioning a Gauss-Newton method by an orthogonal function at each step has never been explored, although some work has been done on conjugate-gradient acceleration for Gauss-Newton methods in the full-rank case (see Ruhe [1979] and Al-Baali and Fletcher [1985]).

3. Studies of Gauss-Newton Methods

Our main concern in this section is with research that specifically addresses computational aspects of Gauss-Newton methods. Comparisons are most often made to Levenberg-Marquardt methods for nonlinear least squares (see, for example, Moré [1978]), and to quasi-Newton methods for unconstrained optimization (see, for example, Dennis and Moré [1977], or any of the references cited above for unconstrained optimization). For a survey of some of the early (mostly theoretical) research on Gauss-Newton methods, see Dennis [1977].

Bard [1970] compares some Gauss-Newton-based methods with a Levenberg-Marquardt method and some quasi-Newton methods for unconstrained optimization on a set of ten test problems from nonlinear parameter estimation. His results are not directly comparable to the Gauss-Newton methods described in this paper, because he uses the eigenvalue decomposition of $J^T J$ in order to solve the normal equations (2.2), and modifies the eigenvalues if their magnitude falls below a certain threshold in order to ensure a positive-definite system. In addition, his implementations include bounds on the variables that are enforced by adding a penalty term to the objective function. He finds that the Gauss-Newton-based methods are more efficient in terms of function and derivative evaluations than the quasi-Newton methods, but that there is no significant difference in the relative performance of the Gauss-Newton-based methods and the Levenberg-Marquardt method.

McKeown [1975a, 1975b] studies test problems of the form,

$$f(x) = f_0 + G_0 x + \frac{1}{2} \begin{pmatrix} x^{\mathrm{T}} H_1 x \\ \vdots \\ x^{\mathrm{T}} H_m x \end{pmatrix},$$

chosen so that factors affecting the rate of convergence could be controlled. He uses three such problems, each with seven different values of a parameter that varies an asymptotic linear convergence factor. The algorithms tested include some quasi-Newton methods for unconstrained optimization, as well as some specialized methods for nonlinear least squares that have since been superseded. He concludes that, when the asympotic convergent factor is small, the Gauss-Newton method is more efficient than the quasi-Newton methods but that the opposite is true when the asympotic convergence factor is large. No mention is made of strategies to deal with rank-deficient Jacobians in the Gauss-Newton method, so that presumably this situation is never encountered in his experiments. We included these problems in our numerical tests (see the results for problems 39 - 41 in the Appendix) and found that the Jacobian matrix was well-conditioned at each iteration in every case.

Ramsin and Wedin [1977] compare the performance of a Gauss-Newton-based method with that of a Levenberg-Marquardt method for nonlinear least squares and a quasi-Newton method for unconstrained optimization, both from the Harwell Library. The quasi-Newton routine required an initial estimate H_0 of the Hessian matrix, and the choice $H_0 = J(x_0)^{\mathrm{T}} J(x_0)$ was made on the basis of preliminary tests that showed equal or better performance compared to $H_0 = I$. The test problems were constructed so that asymptotic properties could be monitored and are similar to those of McKeown [1975a, 1975b] mentioned above. In all cases considered, the Jacobian matrix had full column rank at the solution. The algorithm of Ramsin and Wedin uses the steepest-descent direction, rather than the Gauss-Newton direction, whenever the decrease in the objective is considered unacceptably small. The experiments involved variation of a large number of parameters. Ramsin and Wedin conclude that their Gauss-Newton-based method and the Levenberg-Marquardt method are identical when the asymptotic convergence factor is small, but that the results do not show that either method is consistently better for large asymptotic convergence factors. Also, they find that in instances when the asymptotic convergence factor is large, the quasi-Newton method may be more efficient, although superlinear convergence of the quasi-Newton method was never observed. Ramsin and Wedin maintain that Gauss-Newton should not be used when (i) the current iterate x_k is close to the solution x^*, and the relative

decrease in the size of the gradient is small, when (ii) x_k is not near x^*, and the decrease in the sum of squares relative to the size of the gradient is small, or when (iii) J_k is nearly rank-deficient. Conditions (i) and (ii) are indicators of inefficiency for any minimization algorithm; in general the problem of ascertaining the closeness of an iterate to a minimum is as difficult as solving the original problem. As for condition (iii), we show in Section 5 that rapidly convergent Gauss-Newton methods may exist even if nearly rank-deficient Jacobians are encountered, but that it appears that different rules for estimating the rank of the Jacobian must be applied to different types of nonlinear least-squares problems in order to obtain this favorable behavior.

Deuflhard and Apostolescu [1980] suggest selecting a step length for the Gauss-Newton direction based on decreasing the merit function $\|J_k^\dagger f(x)\|_2$ rather than $\|f(x)\|_2^2$, for a class of nonlinear least-squares problems that includes zero-residual problems. The function $J_k^\dagger$ is the *pseudo-inverse* of J_k (see, for example, Golub and Van Loan [1983], Chapter 6); $J_k^\dagger f_k$ is another way of representing the minimum l_2-norm solution to $\|J_k p + f_k\|_2$. They reason that the Gauss-Newton direction is the steepest-descent direction for the function $\|J_k^\dagger f(x)\|_2^2$, so that the geometry of the level surfaces defined by $\|J_k^\dagger f(x)\|_2^2$ is more favorable to avoiding small steps in the linesearch. A shortcoming of this approach is that is that there are no global convergence results. The merit function depends on x_k, so that a different function is being reduced at each step. Another difficulty is that, although the authors state that numerical experience supports selection of a step length based on $\|J_k^\dagger f(x)\|_2$ for ill-conditioned problems, the transformation $J_k^\dagger$ is not numerically well-defined under these circumstances. Therefore neither the Gauss-Newton search direction, nor the merit function, is numerically well-defined when the columns of J_k are nearly linearly dependent.

Wedin and Lindström [1987] present a hybrid algorithm for nonlinear least-squares that combines a Gauss-Newton method with a finite-difference Newton method. The Gauss-Newton method is implemented with a QR factorization and a scheme for rank estimation that depends on information from the previous iteration, as well as on a user-supplied tolerance. They give numerical results for a set of thirty large-residual test problems constructed by Al-Baali and Fletcher [1985], and compare their results with those given by Al-Baali and Fletcher for two hybrid Gauss-Newton/BFGS methods and a version of NL2SOL. Wedin and Lindström find that their method gives better overall results than the other methods, although their method does fail in three cases due to a finite-difference Hessian that is not positive definite.

Fraley [1987] gives numerical results for a large set of test problems using widely-distributed software for unconstrained optimization and nonlinear least squares. She also includes some Gauss-Newton methods that use LSSOL [Gill et al. (1986a)] to solve the linear least-squares subproblem (these results are reproduced in an appendix to this paper). Her findings confirm that Gauss-Newton methods are often among the best available techniques for nonlinear least squares — especially zero-residual problems — but that there are many cases in which they fail or are inefficient. However, no general *a priori* characterization is given of those problems on which Gauss-Newton will work well; the present paper gives some insight into why it is difficult to do so.

4. Description of Numerical Results

This section gives general information on the numerical results that are presented in the remainder of this paper.

In the examples of Section 5, the LINPACK routine DSVDC [Dongarra et al. (1979)] is used to compute the singular-value decomposition (SVD) of the Jacobian at each iteration; the linear least-squares subproblems within the Gauss-Newton methods are then solved via the SVD. A detailed description of the solution procedure for the subproblems is given in that section. The same procedure is also used for the Gauss-Newton example in Section 6, although rank estimation is not an issue there because the Jacobian is well-conditioned. The linesearch for the Gauss-Newton examples in Sections 5, as well as for all of the numerical results in Section 6, is taken from the nonlinear programming package NPSOL [Gill et al. (1979), (1986b)], and requires both function and gradient evaluations.

The Gauss-Newton methods in Section 5 are compared to numerical results for some unconstrained optimization methods using the following widely-distributed software:

program	method	derivative information	global strategy	source
MNA/E04LBF	modified Newton	second	linesearch	NPL/NAG
NPSOL	quasi-Newton (BFGS)	first	linesearch	SOL/NAG
DMNH/HUMSL	modified Newton	second	trust region	PORT/ACM
DMNG/SUMSL	quasi-Newton (BFGS)	first	trust region	PORT/ACM

These programs come from the following software sources:

NAG	-	Numerical Algorithms Group, Inc.
NPL	-	National Physical Laboratory, England
PORT	-	PORT Mathematical Software Library, A. T. & T. Bell Laboratories, Inc.
ACM	-	Association for Computing Machinery
SOL	-	Systems Optimization Laboratory, Stanford University

The following keywords, listed under the label 'conv.' in the tables, are used to describe abnormal termination conditions:

F LIM.	-	function evaluation limit reached
LOOP	-	subroutine appears to loop
TIME	-	time limit exceeded

In the tables, under the label 'est. err.', we include the quantity

$$\frac{\|f^*\|_2^2 - \|f_{best}\|_2^2}{1 + \|f_{best}\|_2^2},$$

where f^* is the value of f at the point of termination, and $\|f_{best}\|_2$ is the best available estimate of the norm of the solution, in order to get some idea of the error in $\|f^*\|_2$. For those problems that have nonzero residuals, the value of $\|f_{best}\|_2$ is given to six figures of accuracy, rounded down.

We use the notation $rank(J)$ for numerical definitions of the rank of the Jacobian, and $cond(J)$ for the condition number of the Jacobian (the ratio of the largest singular value to the smallest singular value — see, for example, Golub and Van Loan [1983]).

Two sets of data are given for each routine on each example, corresponding to two different sets of values for parameters in the termination criteria. This data is taken from Chapter 2 of Fraley [1987], which contains detailed information about the choices made for the parameter values.

All of the programs were run in FORTRAN using double precision on the IBM 3081 and IBM 3033 computers at Stanford Linear Accelerator Center, for which

$$\text{relative machine precision } \epsilon_M = 2.22\ldots \times 10^{-16}\ ;\ \sqrt{\epsilon_M} = 1.49\ldots \times 10^{-8}.$$

5. Performance on Problems with Ill-Conditioned Jacobians

We explained in Section 2 that the Gauss-Newton framework defines a class of methods, whose members are distinguished by the numerical algorithm for solving the linear least-squares subproblem (2.3) for a search direction, as well as by the linesearch method that is subsequently used to find a steplength along that direction. This section is concerned with the variablity in Gauss-Newton algorithms that is due to computational procedures for the linear least-squares subproblem. The most stable techniques for solving ill-conditioned linear least-squares problems involve orthogonal factorizations: the singular-value decomposition (SVD) and the QR factorization (see the references cited in Section 1 on linear least squares). The linear least-squares subproblems within our Gauss-Newton examples are solved by means of the SVD. Results are not given for Gauss-Newton methods that use the QR factorization, because the same basic considerations apply in choosing the search direction, and also because in practice the behavior is similar to that observed for the SVD.

5.1. SVD Solution to Linear Least-Squares Subproblems

Given the singular-value decomposition of the Jacobian

$$J = \begin{cases} U(S \quad 0)V^T, & \text{if } m < n; \\ USV^T, & \text{if } m = n; \\ U\begin{pmatrix} S \\ 0 \end{pmatrix} V^T, & \text{if } m > n; \end{cases} \tag{5.1}$$

where S is diagonal with non-negative diagonal entries $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min\{m,n\}}$, and U and V are orthogonal, define

$$r_{\max} \equiv \max \{ i \mid \sigma_i \neq 0 \}.$$

Let

$$p_i \equiv \sum_{j=1}^{i} \tau_j v_j; \quad \tau_j \equiv -\frac{u_j^T f}{\sigma_j}; \quad i = 1, 2, \ldots, r_{\max}, \tag{5.2}$$

where u_j, v_j are the jth columns of U and V, respectively. The columns of V form an orthonormal basis for $\Re^n$, and τ_j, $j = 1, 2, \ldots, i$, are the components of p_i in terms of this basis, with

$$\|p_i\|_2^2 = \sum_{j=1}^{i} \tau_j^2.$$

When $i < \min\{m,n\}$, p_i has no component in the space spanned by $\{v_{i+1}, v_{i+2}, \ldots, v_{\min\{m,n\}}\}$. In exact arithmetic, each p_i is either orthogonal to the gradient $\bar{g} \equiv J^T f$ of the nonlinear least-squares objective, or it is a descent direction (see, for example, Chapter 4 of Fraley [1987]).

In practice the SVD cannot be computed exactly, and the solution to the linear least-squares subproblem (2.3) is taken to be p_r, where $r \leq r_{\max}$ is an estimate of the rank of J. In the examples below, the numerical rank of the Jacobian is defined to be

$$rank(J) \equiv \max \{ \, i \mid \sigma_i > \epsilon(1 + \sigma_1) \, \}. \tag{5.3}$$

This criterion depends only on J and does not take into account the size of the search direction p, the angle between p and the gradient, or the vector f. Some specific examples will now be given that show some of the difficulties involved in defining $rank(J)$ for Gauss-Newton methods.

5.2. Chebyquad $n = m = 8$ (# 35a.)

The first example is related to the problem of locating nodes for Chebyschev quadrature [Fletcher (1965); Moré, Garbow, and Hillstrom (1981)], and demonstrates that the choice of ϵ in (5.3) can be critical.

	Gauss-Newton	
	$\epsilon = 10^{-14}$	$\epsilon \leq 10^{-15}$
f, J evals.	147	124
iters.	44	19
$\|x^*\|_2$	1.65	1.63
$\|f^*\|_2$	10^{-2}	10^{-1}
$\|\bar{g}^*\|_2$	10^{-11}	10^{-1}
est. err.	10^{-9}	10^{-2}

The algorithm succeeds in finding an approximate minimum when $\epsilon = 10^{-14}$, although it fails when $\epsilon = 10^{-15}$. The problem is rather easily solved by the unconstrained methods, as shown in the table below.

	MNA		DMNH		NPSOL		DMNG	
f evals.	46	46	14	14	33	35	34	38
J evals.	46	46	11	11	33	35	24	28
iters.	15	15	11	11	19	21	24	27
$\|x^*\|_2$	1.65	1.65	1.65	1.65	1.65	1.65	1.65	1.65
$\|f^*\|_2$	10^{-1}	10^{-1}	10^{-1}	10^{-1}	10^{-1}	10^{-1}	10^{-1}	10^{-1}
$\|\bar{g}^*\|_2$	10^{-10}	10^{-10}	10^{-9}	10^{-9}	10^{-5}	10^{-7}	10^{-5}	10^{-8}
est. err.	10^{-9}	10^{-9}	10^{-9}	10^{-9}	10^{-9}	10^{-9}	10^{-9}	10^{-9}

The next two tables trace the progress of the Gauss-Newton methods for $\epsilon = 10^{-14}$ and $\epsilon = 10^{-15}$, respectively.

Gauss-Newton on Problem **35a.**

$\epsilon = 10^{-14}$

k	f, J evals.	$\|x_k\|_2$	$\|f_k\|_2$	$\|\bar{g}_k\|_2$	$\|p_k\|_2$	$\bar{g}_k^T p_k$	α_k	*cond* J_k	*rank* J_k
0	8	2.E+00	2.E-01	8.E-01	2.E+00	-4.E-02	7.3E-02	10^2	8
1	16	2.E+00	2.E-01	7.E-01	3.E+00	-3.E-02	1.5E-02	10^2	8
2	24	2.E+00	2.E-01	7.E-01	2.E+00	-3.E-02	1.5E-02	10^2	8
3	32	2.E+00	2.E-01	6.E-01	4.E+00	-3.E-02	3.5E-02	10^2	8
4	35	2.E+00	2.E-01	5.E-01	7.E-01	-3.E-02	3.1E-01	10^2	8
5	37	2.E+00	1.E-01	3.E-01	2.E-01	-1.E-02	2.2E-01	10^1	8
6	41	2.E+00	1.E-01	2.E-01	6.E-01	-1.E-02	1.6E-02	10^2	8
7	47	2.E+00	1.E-01	2.E-01	1.E+01	-9.E-03	5.0E-05	10^3	8
8	54	2.E+00	1.E-01	2.E-01	1.E+02	-9.E-03	4.9E-07	10^4	8
9	62	2.E+00	1.E-01	2.E-01	1.E+03	-9.E-03	4.8E-09	10^5	8
10	69	2.E+00	1.E-01	2.E-01	1.E+04	-9.E-03	5.1E-11	10^6	8
11	76	2.E+00	1.E-01	2.E-01	1.E+05	-9.E-03	5.1E-13	10^7	8
12	83	2.E+00	1.E-01	2.E-01	1.E+06	-9.E-03	5.0E-15	10^8	8
13	90	2.E+00	1.E-01	2.E-01	1.E+07	-9.E-03	4.9E-17	10^9	8
14	97	2.E+00	1.E-01	2.E-01	1.E+08	-9.E-03	4.9E-19	10^{10}	8
15	104	2.E+00	1.E-01	2.E-01	1.E+09	-9.E-03	4.7E-21	10^{11}	8
16	111	2.E+00	1.E-01	2.E-01	1.E+10	-9.E-03	4.7E-23	10^{12}	8
17	118	2.E+00	1.E-01	2.E-01	1.E+11	-9.E-03	4.7E-25	10^{13}	8
18	120	2.E+00	1.E-01	2.E-01	8.E-02	-4.E-03	5.7E-01	10^{14}	7
19	123	2.E+00	8.E-02	2.E-01	8.E-03	-8.E-04	2.1E+00	10^{14}	7
20	124	2.E+00	6.E-02	7.E-02	9.E-03	-5.E-04	1.0E+00	10^{14}	7
21	125	2.E+00	6.E-02	3.E-02	2.E-03	-5.E-05	1.0E+00	10^{14}	7
22	126	2.E+00	6.E-02	1.E-02	1.E-03	-1.E-05	1.0E+00	10^{14}	7
23	127	2.E+00	6.E-02	5.E-03	4.E-04	-2.E-06	1.0E+00	10^{14}	7
24	128	2.E+00	6.E-02	2.E-03	2.E-04	-3.E-07	1.0E+00	10^{14}	7
25	129	2.E+00	6.E-02	8.E-04	6.E-05	-4.E-08	1.0E+00	10^{14}	7
26	130	2.E+00	6.E-02	3.E-04	3.E-05	-2.E-09	1.0E+00	10^{14}	7
27	131	2.E+00	6.E-02	1.E-04	1.E-05	-1.E-09	1.0E+00	10^{14}	7
28	132	2.E+00	6.E-02	5.E-05	4.E-06	-2.E-10	1.0E+00	10^{14}	7
29	133	2.E+00	6.E-02	2.E-05	2.E-06	-2.E-11	1.0E+00	10^{14}	7
30	134	2.E+00	6.E-02	8.E-06	6.E-07	-4.E-12	1.0E+00	10^{14}	7
31	135	2.E+00	6.E-02	3.E-06	2.E-07	-6.E-13	1.0E+00	10^{14}	7
32	136	2.E+00	6.E-02	1.E-06	9.E-08	-9.E-14	1.0E+00	10^{14}	7
33	137	2.E+00	6.E-02	5.E-07	4.E-08	-1.E-14	1.0E+00	10^{14}	7
34	138	2.E+00	6.E-02	2.E-07	1.E-08	-2.E-15	1.0E+00	10^{14}	7
35	139	2.E+00	6.E-02	8.E-08	6.E-09	-3.E-16	1.0E+00	10^{14}	7
36	140	2.E+00	6.E-02	3.E-08	2.E-09	-5.E-17	1.0E+00	10^{14}	7
37	141	2.E+00	6.E-02	1.E-08	9.E-10	-8.E-18	1.0E+00	10^{14}	7
38	142	2.E+00	6.E-02	5.E-09	4.E-10	-1.E-18	1.0E+00	10^{14}	7
39	143	2.E+00	6.E-02	2.E-09	1.E-10	-2.E-19	1.0E+00	10^{14}	7
40	144	2.E+00	6.E-02	7.E-10	5.E-11	-3.E-20	1.0E+00	10^{14}	7
41	145	2.E+00	6.E-02	3.E-10	2.E-11	-5.E-21	1.0E+00	10^{14}	7
42	146	2.E+00	6.E-02	1.E-10	8.E-12	-7.E-22	1.0E+00	10^{14}	7
43	147	2.E+00	6.E-02	4.E-11	3.E-12	-1.E-22	1.0E+00	10^{14}	7
		2.E+00	6.E-02	2.E-11					

Gauss-Newton on Problem **35a.**

$\epsilon = 10^{-15}$

k	f, J evals.	$\|x_k\|_2$	$\|f_k\|_2$	$\|\bar{g}_k\|_2$	$\|p_k\|_2$	$\bar{g}_k^T p_k$	α_k	*cond* J_k	*rank* J_k
0	8	2.E+00	2.E-01	8.E-01	2.E+00	-4.E-02	7.3E-02	10^2	8
1	16	2.E+00	2.E-01	7.E-01	3.E+00	-3.E-02	1.5E-02	10^2	8
2	24	2.E+00	2.E-01	7.E-01	2.E+00	-3.E-02	1.5E-02	10^2	8
3	32	2.E+00	2.E-01	6.E-01	4.E+00	-3.E-02	3.5E-02	10^2	8
4	35	2.E+00	2.E-01	5.E-01	7.E-01	-3.E-02	3.1E-01	10^2	8
5	37	2.E+00	1.E-01	3.E-01	2.E-01	-1.E-02	2.2E-01	10^1	8
6	41	2.E+00	1.E-01	2.E-01	6.E-01	-1.E-02	1.6E-02	10^2	8
7	47	2.E+00	1.E-01	2.E-01	1.E+01	-9.E-03	5.0E-05	10^3	8
8	54	2.E+00	1.E-01	2.E-01	1.E+02	-9.E-03	4.9E-07	10^4	8
9	62	2.E+00	1.E-01	2.E-01	1.E+03	-9.E-03	4.8E-09	10^5	8
10	69	2.E+00	1.E-01	2.E-01	1.E+04	-9.E-03	5.1E-11	10^6	8
11	76	2.E+00	1.E-01	2.E-01	1.E+05	-9.E-03	5.1E-13	10^7	8
12	83	2.E+00	1.E-01	2.E-01	1.E+06	-9.E-03	5.0E-15	10^8	8
13	90	2.E+00	1.E-01	2.E-01	1.E+07	-9.E-03	4.9E-17	10^9	8
14	97	2.E+00	1.E-01	2.E-01	1.E+08	-9.E-03	4.9E-19	10^{10}	8
15	104	2.E+00	1.E-01	2.E-01	1.E+09	-9.E-03	4.7E-21	10^{11}	8
16	111	2.E+00	1.E-01	2.E-01	1.E+10	-9.E-03	4.7E-23	10^{12}	8
17	118	2.E+00	1.E-01	2.E-01	1.E+11	-9.E-03	4.7E-25	10^{13}	8
18	124	2.E+00	1.E-01	2.E-01	1.E+12	-9.E-03	0.0E-01	10^{14}	8

Until iteration 18, the Jacobian has full column rank at each step according to (5.3), and it becomes increasingly ill-conditioned as the computation proceeds. The search direction grows very large and approaches orthogonality to the gradient, while the step length decreases. No significant decrease is observed in either $\|f\|_2$ or $\|\bar{g}\|_2$ in iterations 6 - 17. At iteration 18, the two Gauss-Newton methods differ. For $\epsilon = 10^{-14}$, the estimated rank of the Jacobian is reduced to 7, and a significant decrease in the function is achieved. For $\epsilon \leq 10^{-15}$, by (5.3) the Jacobian still has full column rank, and the algorithm terminates because $\alpha_k p_k$ is judged to be negligible relative to $\|x_k\|_2$. Detailed information at the start of iteration 18 for the Gauss-Newton methods is given in the next table.

$\epsilon \leq 10^{-14}$; iteration 18

r	σ_r	$\lvert\tau_r\rvert$	$\lVert p_r\rVert_2$	$\lvert\bar{g}^T p_r\rvert$	$\lvert cos(\bar{g}, p_r)\rvert$
1	10^1	10^{-3}	10^{-3}	10^{-4}	10^0
2	10^1	10^{-16}	10^{-3}	10^{-4}	10^0
3	10^0	10^{-16}	10^{-3}	10^{-4}	10^0
4	10^0	10^{-2}	10^{-2}	10^{-3}	10^0
5	10^0	10^{-15}	10^{-2}	10^{-3}	10^0
6	10^0	10^{-1}	10^{-1}	10^{-3}	10^{-1}
7	10^0	10^{-14}	10^{-1}	10^{-3}	10^{-1}
8	10^{-13}	10^{12}	10^{12}	10^{-2}	10^{-13}

It seems reasonable to say that $rank(J) = 7$ rather than $rank(J) = 8$ at this point, because $\sigma_8 \ll \sigma_7$, $\|p_8\|_7 \gg \|p_7\|_2$, and $|cos(\bar{g}, p_8)| \ll |cos(\bar{g}, p_7)|$. Hence it is not surprising that it is the method with $\epsilon = 10^{-14}$, rather than the one with $\epsilon = 10^{-15}$, that ultimately makes good progress toward the solution.

The behavior of the Gauss-Newton methods can be explained by comparing the sequence $\{p_k^*\}$ of steps from the iterates to the minimum of the function, to the sequence $\{p_k\}$ of Gauss-Newton steps. The magnitudes of the components of these vectors in terms of the basis $\{v_j(x_k)\}$, for iterations 6 - 18, are listed in the tables below.

components $\{\tau_j^*(x_k)\}$ of $p_k^* = x^* - x_k$ in terms of $\{v_j(x_k)\}$

k	$\lvert\tau_1^*\rvert$	$\lvert\tau_2^*\rvert$	$\lvert\tau_3^*\rvert$	$\lvert\tau_4^*\rvert$	$\lvert\tau_5^*\rvert$	$\lvert\tau_6^*\rvert$	$\lvert\tau_7^*\rvert$	$\lvert\tau_8^*\rvert$
6	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-3}
7	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-4}
8	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-5}
9	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-6}
10	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-7}
11	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-8}
12	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-9}
13	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-10}
14	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-11}
15	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-12}
16	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-13}
17	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-14}
18	10^{-2}	10^{-9}	10^{-8}	10^{-2}	10^{-9}	10^{-2}	10^{-9}	10^{-15}

components $\{\tau_j(x_k)\}$ of p_k in terms of $\{v_j(x_k)\}$

k	$\lvert\tau_1\rvert$	$\lvert\tau_2\rvert$	$\lvert\tau_3\rvert$	$\lvert\tau_4\rvert$	$\lvert\tau_5\rvert$	$\lvert\tau_6\rvert$	$\lvert\tau_7\rvert$	$\lvert\tau_8\rvert$
6	10^{-3}	10^{-17}	10^{-16}	10^{-2}	10^{-14}	10^{-1}	10^{-15}	10^{0}
7	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{1}
8	10^{-3}	10^{-17}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{2}
9	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{3}
10	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{4}
11	10^{-3}	10^{-17}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{5}
12	10^{-3}	10^{-17}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{6}
13	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{7}
14	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{8}
15	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{9}
16	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{10}
17	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{11}
18	10^{-3}	10^{-16}	10^{-16}	10^{-2}	10^{-15}	10^{-1}	10^{-14}	10^{12}

The step p_k^* to the minimum approaches orthogonality to $v_8(x_k)$, while the Gauss-Newton search direction becomes dominated by the component in the direction of $v_8(x_k)$ due to the ill-conditioning in the Jacobian. Hence, by iteration 18, p_k is almost orthogonal to p_k^*. The question of when to say that J has rank 7 rather than rank 8 is a difficult one. If full column rank is assumed until the search direction becomes numerically orthogonal to the gradient then the method may become very inefficient (see iterations 6 - 18, where about seven function evaluations are required per iteration). On the other hand, if the step to the minmum has a component in the estimated null space $null(J)$, underestimating $rank(J)$ will inhibit decrease in $null(J)$, because the Gauss-Newton search direction will be orthogonal to $null(J)$.

5.3. Matrix Square Root 1 $n = m = 4$ (# 36a.)

Another instance in which Gauss-Newton methods encounter ill-conditioned Jacobians is the problem of finding the square root of a given (square) matrix (see the Appendix). Although the matrix in question is only of order 2, the problem is a difficult one for the unconstrained methods, as shown in the table below.

	MNA		DMNH		NPSOL		DMNG	
f evals.	4001	4001	4000	4000	786	2618	4000	4000
J evals.	4001	4001	2190	2190	786	2618	2891	2891
iters.	2663	2663	2190	2190	477	1437	2891	2891
$\|\|x^*\|\|_2$	50.4	50.4	17.8	17.8	9.22	10.1	17.0	17.0
$\|\|f^*\|\|_2$	10^{-9}	10^{-9}	10^{-6}	10^{-6}	10^{-5}	10^{-5}	10^{-6}	10^{-6}
$\|\|\bar{g}^*\|\|_2$	10^{-9}	10^{-9}	10^{-6}	10^{-6}	10^{-5}	10^{-7}	10^{-6}	10^{-6}
est. err.	10^{-19}	10^{-19}	10^{-12}	10^{-12}	10^{-9}	10^{-9}	10^{-11}	10^{-11}
conv.	F LIM.	F LIM.	F LIM.	F LIM.			F LIM.	F LIM.

MNA is just Newton's method in this case, since the exact Hessian matrix is never modified, although it does become ill-conditioned, with a condition number of order 10^{11} at the solution. In the Gauss-Newton methods, the Jacobian does becomes ill-conditioned, but unlike the previous problem, a solution is obtained only when the Jacobian is assumed to have full rank at each iteration. A summary of the results for $\epsilon = 10^{-10}$ and $\epsilon \leq 10^{-11}$ are given in the following table.

Gauss-Newton

	$\epsilon = 10^{-10}$	$\epsilon \leq 10^{-11}$
f, J evals.	4004	95
iters.	473	39
$\|\|x^*\|\|_2$	10^1	50.0
$\|\|f^*\|\|_2$	10^{-7}	10^{-16}
$\|\|\bar{g}^*\|\|_2$	10^{-6}	10^{-15}
est. err.	10^{-15}	10^{-33}
conv.	F LIM.	

The next two tables trace the iterations of the Gauss-Newton method for $\epsilon = 10^{-10}$ and $\epsilon = 10^{-11}$, respectively.

Gauss-Newton on Problem **36a.**

$\epsilon = 10^{-10}$

k	f, J evals.	$\|x_k\|_2$	$\|f_k\|_2$	$\|\bar{g}_k\|_2$	$\|p_k\|_2$	$\bar{g}_k^T p_k$	α_k	*cond* J_k	*rank* J_k
0	2	1.E+00	2.E+00	3.E+00	9.E-01	-3.E+00	1.0E+00	10^0	4
1	3	9.E-01	6.E-01	6.E-01	8.E-01	-4.E-01	1.0E+00	10^1	4
2	5	1.E+00	4.E-01	7.E-01	1.E+00	-1.E-01	5.5E-01	10^2	4
3	7	2.E+00	3.E-01	8.E-01	2.E+00	-8.E-02	4.5E-01	10^3	4
4	9	3.E+00	2.E-01	8.E-01	2.E+00	-5.E-02	4.0E-01	10^4	4
5	11	4.E+00	2.E-01	9.E-01	3.E+00	-3.E-02	3.7E-01	10^4	4
6	13	5.E+00	2.E-01	1.E+00	3.E+00	-2.E-02	3.4E-01	10^5	4
7	15	6.E+00	1.E-01	1.E+00	4.E+00	-2.E-02	3.3E-01	10^5	4
8	17	7.E+00	1.E-01	1.E+00	4.E+00	-1.E-02	3.2E-01	10^6	4
9	19	8.E+00	1.E-01	1.E+00	5.E+00	-1.E-02	3.1E-01	10^6	4
10	22	1.E+01	1.E-01	1.E+00	6.E+00	-1.E-02	2.0E-01	10^7	4
11	25	1.E+01	9.E-02	1.E+00	6.E+00	-8.E-03	1.8E-01	10^7	4
12	28	1.E+01	8.E-02	1.E+00	7.E+00	-7.E-03	1.7E-01	10^7	4
13	31	1.E+01	7.E-02	1.E+00	7.E+00	-6.E-03	1.6E-01	10^7	4
14	34	1.E+01	7.E-02	1.E+00	8.E+00	-5.E-03	1.5E-01	10^8	4
15	37	2.E+01	6.E-02	1.E+00	8.E+00	-4.E-03	1.5E-01	10^8	4
16	40	2.E+01	6.E-02	1.E+00	8.E+00	-3.E-03	1.4E-01	10^8	4
17	43	2.E+01	5.E-02	1.E+00	9.E+00	-3.E-03	1.4E-01	10^8	4
18	46	2.E+01	5.E-02	1.E+00	9.E+00	-3.E-03	1.4E-01	10^8	4
19	49	2.E+01	5.E-02	1.E+00	9.E+00	-2.E-03	1.3E-01	10^8	4
20	52	2.E+01	4.E-02	1.E+00	1.E+01	-2.E-03	1.3E-01	10^9	4
21	55	2.E+01	4.E-02	1.E+00	1.E+01	-2.E-03	1.3E-01	10^9	4
22	58	2.E+01	4.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
23	61	3.E+01	4.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
24	64	3.E+01	3.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
25	67	3.E+01	3.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
26	70	3.E+01	3.E-02	1.E+00	1.E+01	-9.E-04	1.4E-01	10^9	4
27	73	3.E+01	3.E-02	1.E+00	1.E+01	-7.E-04	1.4E-01	10^9	4
28	76	3.E+01	3.E-02	1.E+00	1.E+01	-6.E-04	1.5E-01	10^{10}	4
29	79	3.E+01	3.E-02	1.E+00	1.E+01	-6.E-04	1.6E-01	10^{10}	4
30	82	4.E+01	2.E-02	1.E+00	9.E+00	-5.E-04	1.7E-01	10^{10}	4
31	85	4.E+01	2.E-02	1.E+00	9.E+00	-4.E-04	1.9E-01	10^{10}	4
32	86	4.E+01	2.E-02	1.E+00	3.E-04	-3.E-04	1.0E+00	10^{10}	3
33	93	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	2.1E-04	10^{10}	4
34	98	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	9.9E-05	10^{10}	4
35	103	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	9.9E-05	10^{10}	4
36	108	4.E+01	9.E-08	4.E-06	6.E+00	-9.E-15	9.9E-05	10^{10}	4
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
470	3986	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	2.2E-05	10^{10}	4
471	3995	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	2.2E-05	10^{10}	4
472	4004	4.E+01	9.E-08	4.E-06	6.E+00	-8.E-15	2.2E-05	10^{10}	4
		4.E+01	9.E-08	4.E-06					

Gauss-Newton on Problem 36a.

$\epsilon = 10^{-11}$

k	f, J evals.	$\|x_k\|_2$	$\|f_k\|_2$	$\|\bar{g}_k\|_2$	$\|p_k\|_2$	$\bar{g}_k^T p_k$	α_k	$cond\ J_k$	$rank\ J_k$
0	2	1.E+00	2.E+00	3.E+00	9.E-01	-3.E+00	1.0E+00	10^0	4
1	3	9.E-01	6.E-01	6.E 01	8.E-01	-4.E-01	1.0E+00	10^1	4
2	5	1.E+00	4.E-01	7.E-01	1.E+00	-1.E-01	5.5E-01	10^2	4
3	7	2.E+00	3.E-01	8.E-01	2.E+00	-8.E-02	4.5E-01	10^3	4
4	9	3.E+00	2.E-01	8.E-01	2.E+00	-5.E-02	4.0E-01	10^4	4
5	11	4.E+00	2.E-01	9.E-01	3.E+00	-3.E-02	3.7E-01	10^4	4
6	13	5.E+00	2.E-01	1.E+00	3.E+00	-2.E-02	3.4E-01	10^5	4
7	15	6.E+00	1.E-01	1.E+00	4.E+00	-2.E-02	3.3E-01	10^5	4
8	17	7.E+00	1.E-01	1.E+00	4.E+00	-1.E-02	3.2E-01	10^6	4
9	19	8.E+00	1.E-01	1.E+00	5.E+00	-1.E-02	3.1E-01	10^6	4
10	22	1.E+01	1.E-01	1.E+00	6.E+00	-1.E-02	2.0E-01	10^7	4
11	25	1.E+01	9.E-02	1.E+00	6.E+00	-8.E-03	1.8E-01	10^7	4
12	28	1.E+01	8.E-02	1.E+00	7.E+00	-7.E-03	1.7E-01	10^7	4
13	31	1.E+01	7.E-02	1.E+00	7.E+00	-6.E-03	1.6E-01	10^7	4
14	34	1.E+01	7.E-02	1.E+00	8.E+00	-5.E-03	1.5E-01	10^8	4
15	37	2.E+01	6.E-02	1.E+00	8.E+00	-4.E-03	1.5E-01	10^8	4
16	40	2.E+01	6.E-02	1.E+00	8.E+00	-3.E-03	1.4E-01	10^8	4
17	43	2.E+01	5.E-02	1.E+00	9.E+00	-3.E-03	1.4E-01	10^8	4
18	46	2.E+01	5.E-02	1.E+00	9.E+00	-3.E-03	1.4E-01	10^8	4
19	49	2.E+01	5.E-02	1.E+00	9.E+00	-2.E-03	1.3E-01	10^8	4
20	52	2.E+01	4.E-02	1.E+00	1.E+01	-2.E-03	1.3E-01	10^9	4
21	55	2.E+01	4.E-02	1.E+00	1.E+01	-2.E-03	1.3E-01	10^9	4
22	58	2.E+01	4.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
23	61	3.E+01	4.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
24	64	3.E+01	3.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
25	67	3.E+01	3.E-02	1.E+00	1.E+01	-1.E-03	1.3E-01	10^9	4
26	70	3.E+01	3.E-02	1.E+00	1.E+01	-9.E-04	1.4E-01	10^9	4
27	73	3.E+01	3.E-02	1.E+00	1.E+01	-7.E-04	1.4E-01	10^9	4
28	76	3.E+01	3.E-02	1.E+00	1.E+01	-6.E-04	1.5E-01	10^{10}	4
29	79	3.E+01	3.E-02	1.E+00	1.E+01	-6.E-04	1.6E-01	10^{10}	4
30	82	4.E+01	2.E-02	1.E+00	9.E+00	-5.E-04	1.7E-01	10^{10}	4
31	85	4.E+01	2.E-02	1.E+00	9.E+00	-4.E-04	1.9E-01	10^{10}	4
32	87	4.E+01	2.E-02	1.E+00	8.E+00	-3.E-04	3.2E-01	10^{10}	4
33	89	4.E+01	2.E-02	9.E-01	7.E+00	-3.E-04	3.8E-01	10^{10}	4
34	91	4.E+01	1.E-02	8.E-01	5.E+00	-2.E-04	5.3E-01	10^{10}	4
35	92	5.E+01	1.E-02	6.E-01	3.E+00	-1.E-04	1.0E+00	10^{10}	4
36	93	5.E+01	4.E-03	3.E-01	3.E-01	-1.E-05	1.0E+00	10^{11}	4
37	94	5.E+01	1.E-05	7.E-04	6.E-04	-1.E-10	1.0E+00	10^{11}	4
38	95	5.E+01	2.E-11	1.E-09	1.E-09	-4.E-22	1.0E+00	10^{11}	4
		5.E+01	6.E-17	4.E-15					

The first difference between the two methods occurs at iteration 33. Data available from the SVD at the start of the iteration is shown in the following table.

$\epsilon \leq 10^{-10}$; iteration 33

r	σ_r	$\lvert\tau_r\rvert$	$\lVert p_r\rVert_2$	$\lvert\bar{g}^T p_r\rvert$	$\lvert cos(\bar{g}, p_r)\rvert$
1	10^2	10^{-4}	10^{-4}	10^{-4}	10^0
2	10^2	10^{-4}	10^{-4}	10^{-3}	10^0
3	10^{-2}	10^{-15}	10^{-4}	10^{-3}	10^0
4	10^{-8}	10^1	10^1	10^{-3}	10^{-5}

The case for saying that $rank(J) = 3$ appears to be fairly strong. There is a large gap between σ_4 and σ_3, and $|cos(\bar{g}, p_4)|$ is significantly smaller than $|cos(\bar{g}, p_3)|$. Moreover, it would appear that the step taken when $\epsilon = 10^{-10}$ and $rank(J) = 3$ is better, in the sense that the reduction in the values of both $\|f\|_2$ and $\|g\|_2$ is appreciably greater than the reduction achieved when $\epsilon = 10^{-11}$ and $rank(J) = 4$. On the other hand, $|p_4|$ is not especially large for either choice of rank. For $\epsilon = 10^{-10}$, the algorithm subsequently makes unacceptably slow progress, while for $\epsilon = 10^{-11}$, quadratic convergence occurs after a few more iterations.

To see why no further progress can be made for $\epsilon = 10^{-10}$, consider the following table of information on the state of the method at the start of iteration 34.

$\epsilon \leq 10^{-10}$; iteration 34

r	σ_r	$\lvert\tau_r\rvert$	$\lVert p_r\rVert_2$	$\lvert\bar{g}^T p_r\rvert$	$\lvert cos(\bar{g}, p_r)\rvert$
1	10^2	10^{-9}	10^{-4}	10^{-4}	10^0
2	10^2	10^{-9}	10^{-4}	10^{-4}	10^0
3	10^{-2}	10^{-16}	10^{-4}	10^{-4}	10^0
4	10^{-8}	10^1	10^1	10^{-4}	10^{-5}

The singular values are nearly the same as those of the previous iteration, but the change is enough to have $rank(J) = 4$ rather than $rank(J) = 3$ according to (5.3). The value of $\|f\|_2$ has decreased significantly after iteration 33 : $|\tau_1|$ and $|\tau_2|$, which were the dominant components just prior to iteration 33, are much smaller at the start of iteration 34, although $|\tau_3|$ and $|\tau_4|$ are essentially unchanged. As a consequence, $\|p_4\|_2$ is now very large relative to $\|p_3\|_2$, but

$|cos(\bar{g}, p_4)|$ is small since v_4 is close to being orthogonal to g. In fact, if (5.3) is disregarded and $rank(J)$ forced to be 3, the method will converge to a local minimum in one step.

As in the previous section, we compare the sequence $\{p_k^*\}$ of steps from the iterates to the minimum of the function, to the sequence $\{p_k\}$ of Gauss-Newton steps.

components $\{\tau_j^*(x_k)\}$ of $p_k^* = x^* - x_k$ in terms of $\{v_j(x_k)\}$

k	$\lvert\tau_1^*\rvert$	$\lvert\tau_2^*\rvert$	$\lvert\tau_3^*\rvert$	$\lvert\tau_4^*\rvert$
28	10^{-3}	10^{-3}	10^{-15}	10^{1}
29	10^{-3}	10^{-3}	10^{-16}	10^{1}
30	10^{-3}	10^{-3}	10^{-14}	10^{1}
31	10^{-3}	10^{-3}	10^{-14}	10^{1}
32	10^{-3}	10^{-3}	10^{-15}	10^{1}

components $\{\tau_j(x_k)\}$ of p_k in terms of $\{v_j(x_k)\}$

k	$\lvert\tau_1\rvert$	$\lvert\tau_2\rvert$	$\lvert\tau_3\rvert$	$\lvert\tau_4\rvert$
28	10^{-4}	10^{-4}	10^{-15}	10^{1}
29	10^{-4}	10^{-4}	10^{-15}	10^{1}
30	10^{-4}	10^{-4}	10^{-15}	10^{1}
31	10^{-4}	10^{-4}	10^{-14}	10^{1}
32	10^{-4}	10^{-4}	10^{-15}	10^{1}

Taking $rank(J) = 3$ is a bad strategy, in this case, because the solution lies mainly in the direction of $v_4(x_k)$.

5.4. Watson $n = 20$; $m = 31$ (# 20d.)

The final example for this section is a problem that might seem to be very hard for Gauss-Newton methods. In Watson's problem [Brent (1973); Moré, Garbow, and Hillstrom (1981)], a polynomial of degree n is fitted to approximate the solution of an ordinary differential equation. The Jacobian matrix for $n = 20$ has singular values of order 10^2, 10^1, 10^1, 10^0, 10^0, 10^0, 10^{-1}, 10^{-1}, 10^{-2}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}, 10^{-9} 10^{-11}, and 10^{-12} at the origin. Yet there is very little difficulty in obtaining a solution, starting from $x_0 = 0$, for a wide range of values of ϵ, as shown in the table below.

Gauss-Newton

ϵ	10^{-8}	10^{-9}	10^{-10}	$10^{-11}; 10^{-12}$	10^{-13}	$\geq 10^{-14}$
f. J evals.	6	6	6	6	6	6
iters.	5	5	5	5	5	5
$\|x^*\|_2$	1.07	1.11	1.55	5.21	29.2	247.
$\|f^*\|_2$	10^{-8}	10^{-8}	10^{-9}	10^{-9}	10^{-10}	10^{-10}
$\|\bar{g}^*\|_2$	10^{-14}	10^{-14}	10^{-14}	10^{-12}	10^{-14}	10^{-12}

Gauss-Newton compares favorably on this problem with results for the unconstrained methods, which are summarized in the next table.

	MNA		DMNH		NPSOL		DMNG	
f evals.	(352)	(251)	50	(149)	76	200	110	134
J evals.	(352)	(251)	27	(56)	76	200	108	119
iters.	(189)	(135)	26	(55)	38	99	107	119
$\|x^*\|_2$	10^6	10^6	1.10	1.16	1.06	1.06	1.06	1.06
$\|f^*\|_2$	10^{-3}	10^{-3}	10^{-8}	10^{-8}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
$\|\bar{g}^*\|_2$	10^{-5}	10^{-5}	10^{-13}	10^{-13}	10^{-5}	10^{-8}	10^{-11}	10^{-12}
est. err.	10^{-5}	10^{-5}	10^{-16}	10^{-16}	10^{-8}	10^{-11}	10^{-12}	10^{-13}
conv.	TIME	TIME		LOOP				

In MNA, the Hessian matrix is nearly singular (but not indefinite) at every iteration, with condition number ranging from 10^{11} to 10^{15}, and it is modified at every step. The trust-region algorithm DMNH, which also uses exact second derivatives, loops for some values of the parameters in the termination criteria.

Watson's problem has a number of local minima, so that the value of the Gauss-Newton solution is dependent on ϵ. Nothing can be said concerning which of the local minima is the "better" one without knowing how the solution is going to be used. For the larger values of ϵ, solutions are obtained that are small in magnitude and hence closer to the starting value, because lower values of the rank restrict the size of the search directions. On the other hand, the final value of the sum of squares is smaller for smaller values of ϵ, because the objective function is being decreased in a larger subspace at each step. Details of the Gauss-Newton iterations are given below.

Gauss-Newton on Problem **20d.**

k	f, J evals.	$\|x_k\|_2$	$\|f_k\|_2$	$\|\bar{g}_k\|_2$	$\|p_k\|_2$	$\bar{g}_k^T p_k$	α_k	*cond* J_k	*rank* J_k
				$\epsilon = 10^{-8}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	15
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	15
2	4	1.E+00	4.E-01	2.E+01	5.E-02	-2.E-01	1.0E+00	10^{13}	15
3	5	1.E+00	2.E-03	1.E-01	5.E-02	-4.E-06	1.0E+00	10^{13}	15
4	6	1.E+00	3.E-08	5.E-07	3.E-05	-2.E-16	1.0E+00	10^{13}	15
		1.E+00	3.E-08	2.E-14					
				$\epsilon = 10^{-9}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	16
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	16
2	4	1.E+00	4.E-01	2.E+01	1.E-01	-2.E-01	1.0E+00	10^{13}	16
3	5	1.E+00	2.E-03	1.E-01	2.E-01	-4.E-06	1.0E+00	10^{13}	16
4	6	1.E+00	2.E-08	5.E-07	1.E-04	-2.E-16	1.0E+00	10^{13}	16
		1.E+00	1.E-08	7.E-15					
				$\epsilon = 10^{-10}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	17
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	17
2	4	1.E+00	4.E-01	2.E+01	5.E-01	-2.E-01	1.0E+00	10^{13}	17
3	5	1.E+00	2.E-03	1.E-01	7.E-01	-4.E-06	1.0E+00	10^{13}	17
4	6	2.E+00	1.E-08	5.E-07	6.E-04	-2.E-16	1.0E+00	10^{13}	17
		2.E+00	4.E-09	2.E-14					
				$\epsilon = 10^{-11}; 10^{-12}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	18
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	18
2	4	1.E+00	4.E-01	2.E+01	2.E+00	-2.E-01	1.0E+00	10^{13}	18
3	5	2.E+00	2.E-03	1.E-01	3.E+00	-4.E-06	1.0E+00	10^{13}	18
4	6	5.E+00	1.E-08	5.E-07	4.E-03	-2.E-16	1.0E+00	10^{13}	18
		5.E+00	1.E-09	6.E-13					
				$\epsilon = 10^{-13}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	19
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	19
2	4	1.E+00	4.E-01	2.E+01	1.E+01	-2.E-01	1.0E+00	10^{13}	19
3	5	1.E+00	2.E-03	1.E-01	2.E+01	-4.E-06	1.0E+00	10^{13}	19
4	6	3.E+00	1.E-08	5.E-07	3.E-02	-2.E-16	1.0E+00	10^{13}	19
		3.E+00	5.E-10	3.E-14					
				$\epsilon = 10^{-14}$					
0	2	0.E+00	5.E+00	2.E+02	1.E+00	-3.E+01	1.0E+00	10^{14}	20
1	3	1.E+00	3.E+00	1.E+02	4.E-01	-6.E+00	1.0E+00	10^{13}	20
2	4	1.E+00	4.E-01	2.E+01	8.E+01	-2.E-01	1.0E+00	10^{13}	20
3	5	8.E+01	2.E-03	1.E-01	2.E+02	-4.E-06	1.0E+00	10^{13}	20
4	6	2.E+02	1.E-08	5.E-07	3.E-01	-2.E-16	1.0E+00	10^{13}	20
		2.E+02	2.E-10	4.E-12					

The condition number of the Jacobian remains very large throughout, yet the search direction is never especially large regardless of the choice of rank, because the sequence $\{|u_i^T f|\}$ is monotonically decreasing at about the same rate as the singular values (see (5.2). The unit step gives sufficient decrease in every instance, on account of the many local minima. Moreover, there is superlinear convergence for each value of ϵ, despite the fact that p becomes very close to being orthogonal to the gradient, with $|cos(\bar{g}, p)|$ ranging from 10^{-5} for $\epsilon = 10^{-8}$, to 10^{-9} for $\epsilon \geq 10^{-14}$ in the final step.

6. An Example of Poor Performance on a Well-Conditioned Zero-Residual Problem

On problems with well-conditioned Jacobians, Gauss-Newton methods are globally convergent, and they are locally quadratically convergent if in addition the residuals vanish at the solution (see Section 2). It is generally believed that Gauss-Newton methods will work well on zero- or small-residual problems in which the Jacobian is never ill-conditioned. In this section, we exhibit a zero-residual problem on which Gauss-Newton performs poorly, although $cond(J_k)$ never exceeds 5×10^3. The example used is the following modification of Rosenbrock's Function [Moré, Garbow, and Hillstrom (1981), p. 21].

Modified Rosenbrock Function $n = m = 2$

$$\phi_1(x) = 100(x_2 - x_1^2)$$

$$\phi_2(x) = 1 - x_1$$

$$x_0 = (0, 0)$$

$$f(x) = \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ at } (1, 1)$$

The starting point $(0, 0)$ lies at the bottom of a curved steep-sided valley in which the solution $(1, 1)$ also lies. The following table gives the results for Gauss-Newton and Newton's method on this problem.

Modified Rosenbrock $n = m = 2$; $x_0 = (0, 0)$

	Gauss-Newton	Newton's Method
f, J evals.	467	77
iters.	100	50
$\|x^*\|_2$	1.41	1.41
$\|f^*\|_2$	10^{-15}	10^{-13}
$\|\bar{g}^*\|_2$	10^{-13}	10^{-12}
est. err.	10^{-30}	10^{-26}

The same linesearch is used here for both methods (see Section 4). Newton's method can be applied without modification, since the Hessian, as well as the Jacobian, is well-conditioned. In this case, Gauss-Newton is Newton's method for nonlinear equations, because $n = m$. Contour plots of the progress of the two methods are displayed on the pages following Section 7 of this paper.

The minimum of the Gauss-Newton model (2.1) lies well outside the valley in which the starting value and minimum are located, at least until the iterates are very close to the solution. The univariate function $\Phi(\alpha) = \|f(x_k + \alpha p_k)\|_2^2$ actually has a maximum at $\alpha = 1$ for $\alpha \in [0, 1]$, rather than a minimum as predicted by the quadratic model; moreover, the function rises very steeply from the valley floor to the maximum. Hence a significant number of function evaluations are required in the linesearch in order to minimize $\Phi(\alpha)$, and, initially, rather small steps are taken along the search directions. Strategies for improving the efficiency of the method include decreasing the maximum steplength $\alpha^{\max}$ and relaxing the parameter η that controls the accuracy of the univariate minimization in the linesearch (see, for example, Gill, Murray, and Wright [1981]). For example, if N_k is the number of function evaluations required to determine α_k, and the following scheme is used to define $\alpha_k^{\max}$

$$\alpha_k^{\max} = \gamma_k(1 + \|x_k\|_2)$$

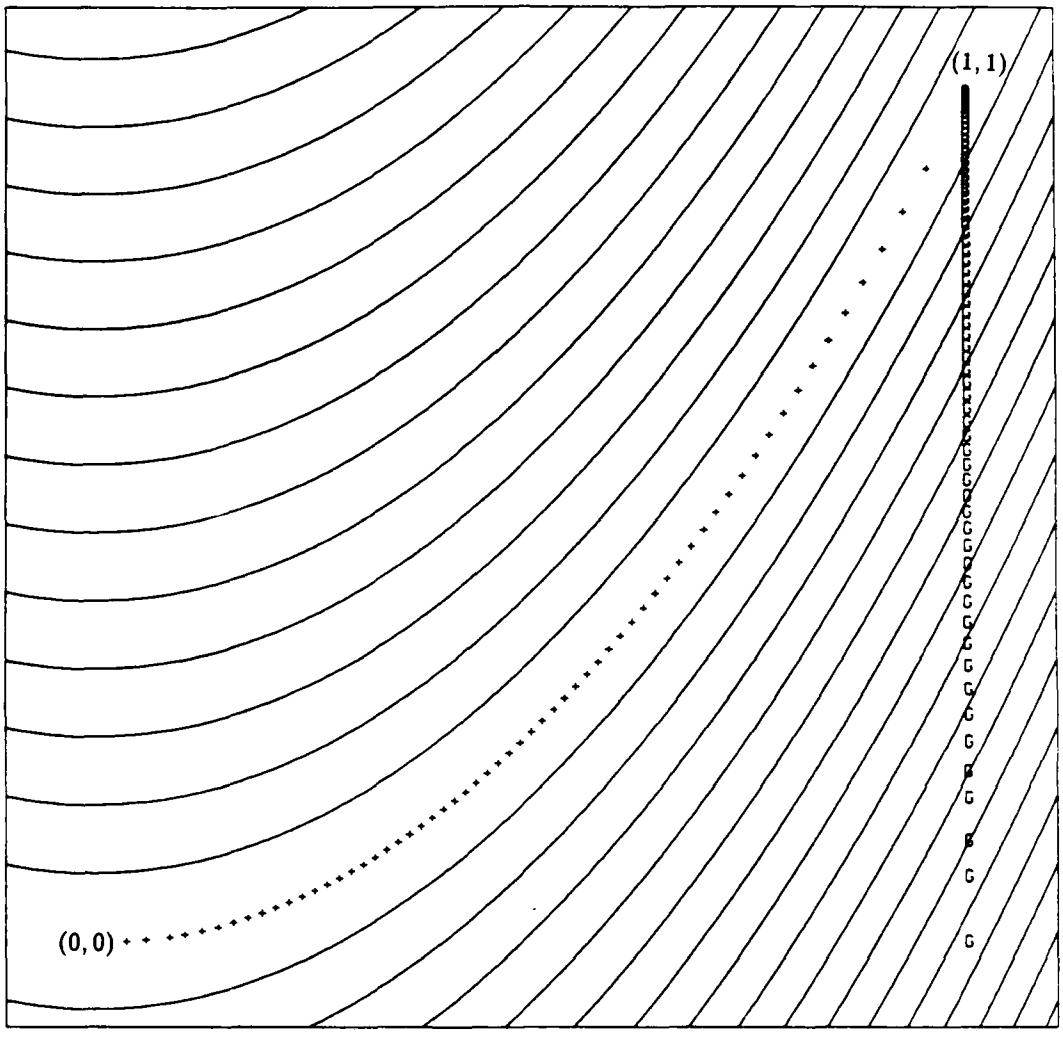
$$\gamma_0 = 1.0$$

$$\gamma_k = \begin{cases} 2\gamma_{k-1} & \text{if } \alpha_{k-1} = \alpha_{k-1}^{\max} \\ \gamma_{k-1} & \text{if } \alpha_{k-1} \neq \alpha_{k-1}^{\max} \text{ and } N_{k-1} \leq 2 \\ \gamma_{k-1}/2 & \text{if } \alpha_{k-1} \neq \alpha_{k-1}^{\max} \text{ and } N_{k-1} > 2, \end{cases}$$

then the Gauss-Newton method solves the problem in only 63 iterations and 135 function evaluations with $\eta = 0.5$. By contrast, the relatively efficient performance of Newton's method can be explained by the fact that the minimum of the Newton quadratic model falls very near the curve along the valley floor connecting $(0,0)$ to $(1,1)$ (which is followed by the iterates of both methods), at all iterations except the first one.

7. Conclusions

We have examined the performance of some Gauss-Newton methods on specific examples and given precise explanations of the observed results in every case. From some of these examples, we conclude that ill-conditioning in the Jacobian does not necessarily imply that a Gauss-Newton method will not work well, but that there appears to be no strategy that is uniformly best for estimating rank in the linear-least squares subproblems. We give another example showing that Gauss-Newton methods may not necessarily be effective on well-conditioned zero-residual problems. Most importantly, we have demonstrated that it is necessary to look at details of the performance of Gauss-Newton methods in order to make meaningful statements about their behavior.



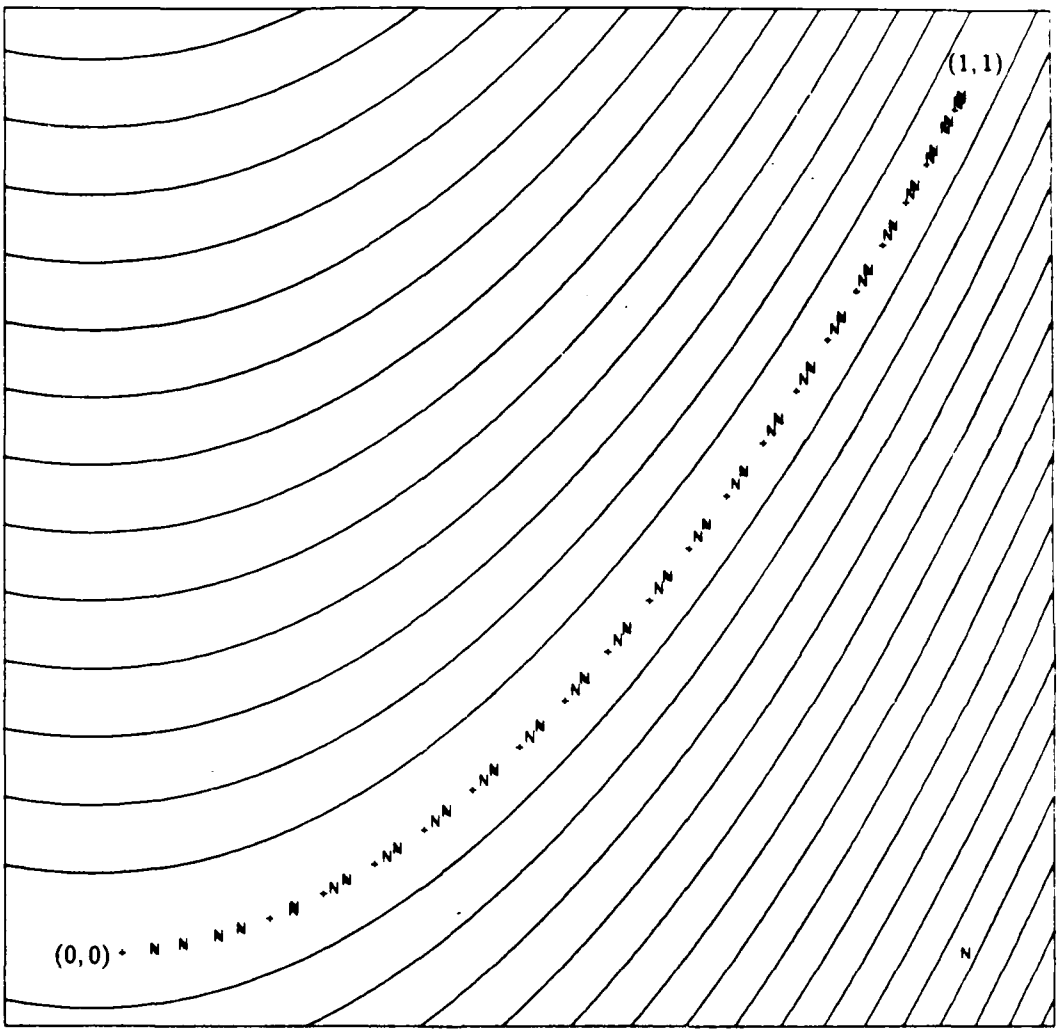
Gauss-Newton Method on the Modified Rosenbrock Function

starting value : $x_0 = (0, 0)$

solution : $x^* = (1, 1)$

G - $x_k + p_k$

\+ - $x_k + \alpha_k p_k$



Newton's Method on the Modified Rosenbrock Function

starting value : $x_0 = (0, 0)$

solution : $x^* = (1, 1)$

N - $x_k + p_k$

\+ - $x_k + \alpha_k p_k$

8. Appendix: Numerical Results for some Gauss-Newton Methods

8.1. Software and Algorithm

In this section numerical results are given for the test problems described in the previous subsection. The software package LSSOL [Gill et al. (1986a)] is used to solve the linear least-squares subproblem (2.3). The linesearch procedure used for the numerical examples in this section, and also in Sections 5 and 6, requires both function and gradient information. It is taken from the nonlinear programming code NPSOL [Gill et al. (1979); (1986b)]. Numerical results for the same set of test problems using widely-distributed software for unconstrained optimization and nonlinear least squares can be found in Fraley [1987].

8.2. Parameters

Parameters in LSSOL were kept at their default values with the following exceptions :

Rank Tolerance	-	varied, see tables
Infinite Bound Size	-	10^{20}

See Gill et al. [1986a] for details concerning the parameters.

In addition, the following parameters are chosen for the linesearch :

η	-	0.5
$\alpha_{\max}$	-	$\min\{(100(1+\|x\|_2)+1)/\|p\|_2, 10^{20}\}$ †

† In some cases the default value $\alpha_{\max}$ was too large and overflow occurred during function evaluation in the linesearch. These cases are indicated in the tables by giving the value $\gamma < 100$ such that $\alpha_{\max} = \min\{(\gamma(1+\|x\|_2)+1)/\|p\|_2, 10^{20}\}$ that was subsequently used to obtain the results in the column labeled "step fac.".

See, for example, Gill, Murray, and Wright [1981] for a discussion of the linesearch parameters.

8.3. Convergence Criteria

Convergence is judged to have occurred at the kth iterate if either

$$\|f_k\|_2 \leq \epsilon_M^{0.9} \tag{8.1}$$

or

$$\|\bar{g}_k\|_2 \leq \epsilon_M^{2/3}(1 + \|f_k\|_2). \tag{8.2}$$

The algorithm is also terminated if there is a negligible change in x,

$$\alpha_k \|p_k\|_2 \leq \epsilon_M^{0.9}(1 + \|x_k\|_2), \tag{8.3}$$

where α_k is the step length determined by the linesearch.

8.4. Table Information

Under the label 'conv.', the following notation is used to describe conditions under which the algorithm terminates :

ABS F	-	(8.1)
G	-	(8.2)
X	-	(8.3)
F LIM	-	function evaluation limit reached

Under the label 'est. err.', we include the quantity

$$\frac{\|f^*\|_2^2 - \|f_{best}\|_2^2}{1 + \|f_{best}\|_2^2}, \tag{8.4}$$

where f^* is the value of f at the point of termination, and $\|f_{best}\|_2$ is the best available estimate of the norm of the solution, in order to get some idea of the error in $\|f^*\|_2$. For those problems that have nonzero residuals, the value of $\|f_{best}\|_2$ is given to six figures of accuracy, rounded down.

A superscript ^{0} following a problem number indicates a zero-residual problem.

A superscript ^{L} following a problem number denotes a linear least-squares problem.

For further details on the numerical tests, see Section 4. Information on the test problems is given in the next section.

Numerical Results for the Gauss-Newton Methods

	n	m	rank tol.	step fac.	f, J evals.	iters.	$\|x^*\|_2$	$\|f^*\|_2$	$\|\bar{g}^*\|_2$	est. err.	conv.
1.^{0}	2	2	1.49×10^{-8}		34	13	1.41	10^{-16}	10^{-15}	10^{-32}	ABS F, G
			2.23×10^{-16}		34	13	1.41	10^{-16}	10^{-15}	10^{-32}	ABS F, G
2.^{0}	2	2	1.49×10^{-8}		138	33	11.4	10^{1}	10^{-6}	10^{1}	X
			2.23×10^{-16}		225	38	11.4	10^{1}	10^{-13}	10^{1}	G
3.^{0}	2	2	1.49×10^{-8}		31	16	7.22	10^{-8}	10^{-7}	10^{-7}	X
			2.23×10^{-16}		44	24	9.11	10^{-16}	10^{-11}	10^{-33}	ABS F, G
4.^{0}	2	3	1.49×10^{-8}		56	14	10^{6}	10^{-22}	10^{-22}	10^{-44}	ABS F, G, X
			2.23×10^{-16}		56	14	10^{6}	10^{-22}	10^{-22}	10^{-44}	ABS F, G X
5.^{0}	2	3	1.49×10^{-8}		8	6	3.04	10^{-14}	10^{-13}	10^{-28}	G
			2.23×10^{-16}		8	6	3.04	10^{-14}	10^{-13}	10^{-28}	G
6.	2	10	1.49×10^{-8}	5.0	1180	166	.365	10^{1}	10^{-6}	10^{-6}	X
			2.23×10^{-16}	5.0	154	22	.501	10^{2}	10^{4}	10^{1}	X
7.^{0}	3	3	1.49×10^{-8}		13	10	1.00	10^{-24}	10^{-23}	10^{-48}	ABS F, G
			2.23×10^{-16}		13	10	1.00	10^{-24}	10^{-23}	10^{-48}	ABS F, G
8.	3	15	1.49×10^{-8}		7	6	2.60	10^{-1}	10^{-11}	10^{-8}	G
			2.23×10^{-16}		7	6	2.60	10^{-1}	10^{-11}	10^{-8}	G
9.	3	15	1.49×10^{-8}		3	2	1.08	10^{-4}	10^{-12}	10^{-14}	G
			2.23×10^{-16}		3	2	1.08	10^{-4}	10^{-12}	10^{-14}	G
10.	3	16	1.49×10^{-8}		87	21	10^{4}	10^{1}	10^{0}	10^{1}	X
			2.23×10^{-16}		30	10	10^{4}	10^{1}	10^{-3}	10^{-7}	X
11.^{0}	3	10	1.49×10^{-8}		(3000)	(1232)	252.	10^{-1}	10^{3}	10^{-2}	F LIM
			2.23×10^{-16}		(3000)	(998)	295.	10^{-1}	10^{-1}	10^{-2}	F LIM.
12.^{0}	3	10	1.49×10^{-8}		7	6	10.1	10^{-16}	10^{-16}	10^{-33}	ABS F, G
			2.23×10^{-16}		7	6	10.1	10^{-16}	10^{-16}	10^{-33}	ABS F, G
13.^{0}	4	4	1.49×10^{-8}		16	15	10^{-5}	10^{-8}	10^{-11}	10^{-16}	G
			2.23×10^{-16}		16	15	10^{-5}	10^{-8}	10^{-11}	10^{-16}	G
14.^{0}	4	6	1.49×10^{-8}		96	40	2.00	10^{-14}	10^{-13}	10^{-29}	ABS F, G
			2.23×10^{-16}		96	40	2.00	10^{-14}	10^{-13}	10^{-29}	ABS F, G
15.	4	11	1.49×10^{-8}		26	12	.328	10^{-2}	10^{-11}	10^{-9}	G
			2.23×10^{-16}		26	12	.328	10^{-2}	10^{-11}	10^{-9}	G
16.	4	20	1.49×10^{-8}		3484	1692	17.6	10^{2}	10^{-8}	10^{-8}	X
			2.23×10^{-16}		3484	1692	17.6	10^{2}	10^{-8}	10^{-8}	X
17.	5	33	1.49×10^{-8}		13	9	2.46	10^{-2}	10^{-11}	10^{-11}	G
			2.23×10^{-16}		13	9	2.46	10^{-2}	10^{-11}	10^{-11}	G
18.^{0}	6	13	1.49×10^{-8}	10.0	(6005)	(770)	2.97	10^{0}	10^{0}	10^{0}	F LIM.
			2.23×10^{-16}		(6006)	(750)	56.6	10^{0}	10^{0}	10^{0}	F LIM.
19.	11	65	1.49×10^{-8}		24	16	9.38	10^{-1}	10^{-11}	10^{-8}	G
			2.23×10^{-16}		24	16	9.38	10^{-1}	10^{-11}	10^{-8}	G

Numerical Results for the Gauss-Newton Methods

	n	m	rank tol.	step fac.	f, J evals.	iters.	$\|x^*\|_2$	$\|f^*\|_2$	$\|\bar{g}^*\|_2$	est. err.	conv.
20a.	6	31	1.49×10^{-8}		12	11	2.44	10^{-2}	10^{-11}	10^{-10}	G
			2.23×10^{-16}		12	11	2.44	10^{-2}	10^{-11}	10^{-10}	G
20b.	9	31	1.49×10^{-8}		6	5	6.06	10^{-3}	10^{-11}	10^{-13}	G
			2.23×10^{-16}		6	5	6.06	10^{-3}	10^{-11}	10^{-13}	G
20c.	12	31	1.49×10^{-8}		6	5	16.6	10^{-5}	10^{-13}	10^{-16}	G
			2.23×10^{-16}		6	5	16.6	10^{-5}	10^{-13}	10^{-16}	G
20d.	20	31	1.49×10^{-8}		6	5	1.07	10^{-8}	10^{-13}	10^{-15}	G
			2.23×10^{-16}		6	5	247.	10^{-10}	10^{-12}	10^{-26}	G
21a.^{0}	10	10	1.49×10^{-8}		34	13	3.16	10^{-16}	10^{-14}	10^{-31}	ABS F, G
			2.23×10^{-16}		34	13	3.16	10^{-16}	10^{-14}	10^{-31}	ABS F, G
21b.^{0}	20	20	1.49×10^{-8}		34	13	4.47	10^{-16}	10^{-14}	10^{-31}	ABS F, G
			2.23×10^{-16}		34	13	4.47	10^{-16}	10^{-14}	10^{-31}	ABS F, G
22a.^{0}	12	12	1.49×10^{-8}		16	15	10^{-4}	10^{-8}	10^{-11}	10^{-15}	G
			2.23×10^{-16}		16	15	10^{-4}	10^{-8}	10^{-11}	10^{-15}	G
22b.^{0}	20	20	1.49×10^{-8}		16	15	10^{-4}	10^{-8}	10^{-11}	10^{-15}	G
			2.23×10^{-16}		16	15	10^{-4}	10^{-8}	10^{-11}	10^{-15}	G
23a.	4	5	1.49×10^{-8}		86	43	.500	10^{-3}	10^{-14}	10^{-10}	G
			2.23×10^{-16}		86	43	.500	10^{-3}	10^{-14}	10^{-10}	G
23b.	10	11	1.49×10^{-8}		99	36	.500	10^{-2}	10^{-12}	10^{-11}	G
			2.23×10^{-16}		99	36	.500	10^{-2}	10^{-12}	10^{-11}	G
24a.	4	8	1.49×10^{-8}		781	204	.759	10^{-3}	10^{-12}	10^{-11}	G
			2.23×10^{-16}		781	204	.759	10^{-3}	10^{-12}	10^{-11}	G
24b.	10	20	1.49×10^{-8}		(10002)	(1636)	.594	10^{-2}	10^{-1}	10^{-4}	F LIM.
			2.23×10^{-16}		(10002)	(1636)	.594	10^{-2}	10^{-1}	10^{-4}	F LIM.
25a.^{0}	10	12	1.49×10^{-8}		11	10	3.16	10^{-15}	10^{-14}	10^{-30}	ABS F, G
			2.23×10^{-16}		11	10	3.16	10^{-15}	10^{-14}	10^{-30}	ABS F, G
25b.^{0}	20	22	1.49×10^{-8}		13	12	4.47	10^{-15}	10^{-13}	10^{-30}	ABS F, G
			2.23×10^{-16}		13	12	4.47	10^{-15}	10^{-13}	10^{-30}	ABS F, G
26a.^{0}	10	10	1.49×10^{-8}		16	8	.306	10^{-11}	10^{-11}	10^{-22}	G
			2.23×10^{-16}		16	8	.306	10^{-11}	10^{-11}	10^{-22}	G
26b.^{0}	20	20	1.49×10^{-8}		25	10	.222	10^{-11}	10^{-11}	10^{-22}	G
			2.23×10^{-16}		25	10	.222	10^{-11}	10^{-11}	10^{-22}	G
27a.^{0}	10	10	1.49×10^{-8}		21	7	3.18	10^{-15}	10^{-14}	10^{-29}	ABS F, G
			2.23×10^{-16}		21	7	3.18	10^{-15}	10^{-14}	10^{-29}	ABS F, G
27b.^{0}	20	20	1.49×10^{-8}	10.0	22	9	4.47	10^{-12}	10^{-11}	10^{-23}	G
			2.23×10^{-16}	10.0	22	9	4.47	10^{-12}	10^{-12}	10^{-23}	G
28a.^{0}	10	10	1.49×10^{-8}		4	3	.412	10^{-15}	10^{-16}	10^{-31}	ABS F, G
			2.23×10^{-16}		4	3	.412	10^{-15}	10^{-16}	10^{-31}	ABS F, G
28b.^{0}	20	20	1.49×10^{-8}		4	3	.571	10^{-16}	10^{-16}	10^{-32}	ABS F, G
			2.23×10^{-16}		4	3	.571	10^{-16}	10^{-16}	10^{-32}	ABS F, G

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	n	m	rank tol.	step fac.	f, J evals.	iters.	$\|x^*\|_2$	$\|f^*\|_2$	$\|\bar{g}^*\|_2$	est. err.	conv.
29a.^{0}	10	10	1.49×10^{-8}		4	3	.412	10^{-14}	10^{-14}	10^{-29}	ABS. F, G
			2.23×10^{-16}		4	3	.412	10^{-14}	10^{-14}	10^{-29}	ABS. F, G
29b.^{0}	20	20	1.49×10^{-8}		4	3	.571	10^{-14}	10^{-14}	10^{-28}	G
			2.23×10^{-16}		4	3	.571	10^{-14}	10^{-14}	10^{-28}	G
30a.^{0}	10	10	1.49×10^{-8}		6	5	2.05	10^{-16}	10^{-15}	10^{-31}	ABS. F, G
			2.23×10^{-16}		6	5	2.05	10^{-16}	10^{-15}	10^{-31}	ABS. F, G
30b.^{0}	20	20	1.49×10^{-8}		6	5	3.04	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
			2.23×10^{-16}		6	5	3.04	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
31a.^{0}	10	10	1.49×10^{-8}		7	6	1.80	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
			2.23×10^{-16}		7	6	1.80	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
31b.^{0}	20	20	1.49×10^{-8}		7	6	2.66	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
			2.23×10^{-16}		7	6	2.66	10^{-15}	10^{-15}	10^{-31}	ABS. F, G
32.^{L}	10	20	1.49×10^{-8}		2	1	3.16	10^{0}	10^{-14}	0.00	G
			2.23×10^{-16}		2	1	3.16	10^{0}	10^{-14}	0.00	G
33.^{L}	10	20	1.49×10^{-8}		3	2	5.40	10^{0}	10^{-10}	10^{-6}	G, X
			2.23×10^{-16}		8	8	10^{13}	10^{0}	10^{2}	10^{-3}	$g^Tp \geq 0$
34.^{L}	10	20	1.49×10^{-8}		3	2	4.90	10^{0}	10^{-11}	10^{-6}	G, X
			2.23×10^{-16}		3	2	4.90	10^{0}	10^{-11}	10^{-6}	G, X
35a.	8	8	1.49×10^{-8}		222	60	1.65	10^{-1}	10^{-11}	10^{-9}	G
			2.23×10^{-16}		110	17	1.63	10^{-1}	10^{-1}	10^{-2}	X
35b.^{0}	9	9	1.49×10^{-8}		107	21	1.73	10^{-16}	10^{-15}	10^{-31}	ABS. F, G
			2.23×10^{-16}		257	37	1.70	10^{-1}	10^{0}	10^{-2}	X
35c.	10	10	1.49×10^{-8}		(10003)	1261	1.79	10^{-1}	10^{-1}	10^{-2}	F LIM
			2.23×10^{-16}		203	28	1.79	10^{-1}	10^{0}	10^{-2}	X
36a.^{0}	4	4	1.49×10^{-8}		(4001)	(677)	17.2	10^{-6}	10^{-4}	10^{-11}	F LIM.
			2.23×10^{-16}		95	39	50.0	10^{-16}	10^{-15}	10^{-33}	ABS. F, G
36b.^{0}	9	9	1.49×10^{-8}		1840	273	18.8	10^{-6}	10^{-12}	10^{-12}	G
			2.23×10^{-16}		92	38	50.0	10^{-16}	10^{-15}	10^{-33}	ABS. F, G
36c.^{0}	9	9	1.49×10^{-8}		20	19	1.73	10^{-11}	10^{-11}	10^{-22}	G
			2.23×10^{-16}		20	19	1.73	10^{-11}	10^{-11}	10^{-22}	G
36d.^{0}	9	9	1.49×10^{-8}		1793	268	19.0	10^{-6}	10^{-11}	10^{-12}	G
			2.23×10^{-16}		(9002)	(1158)	343.	10^{-6}	10^{-5}	10^{-13}	F LIM.
37.	2	16	1.49×10^{-8}		37	35	8.85	10^{1}	10^{-8}	10^{-6}	X
			2.23×10^{-16}		37	35	8.85	10^{1}	10^{-8}	10^{-6}	X
38.	3	16	1.49×10^{-8}		31	24	26.1	10^{1}	10^{-10}	10^{-6}	G
			2.23×10^{-16}		31	24	26.1	10^{1}	10^{-10}	10^{-6}	G

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	n	m	rank tol.	step fac.	f, J evals.	iters.	$\|x^*\|_2$	$\|f^*\|_2$	$\|\bar{g}^*\|_2$	est err.	conv.
39a.	2	3	1.49×10^{-8}		8	7	10^{-6}	10^{-1}	10^{-11}	10^{-7}	G
			2.23×10^{-16}		8	7	10^{-6}	10^{-1}	10^{-11}	10^{-7}	G
39b.	2	3	1.49×10^{-8}		10	7	10^{-7}	10^{-1}	10^{-11}	10^{-7}	G
			2.23×10^{-16}		10	7	10^{-7}	10^{-1}	10^{-11}	10^{-7}	G
39c.	2	3	1.49×10^{-8}		23	14	10^{-7}	10^{-1}	10^{-12}	10^{-7}	G
			2.23×10^{-16}		23	14	10^{-7}	10^{-1}	10^{-12}	10^{-7}	G
39d.	2	3	1.49×10^{-8}		699	343	10^{-7}	10^{-1}	10^{-11}	10^{-7}	G
			2.23×10^{-16}		699	343	10^{-7}	10^{-1}	10^{-11}	10^{-7}	G
39e.	2	3	1.49×10^{-8}		1962	951	10^{-7}	10^{-1}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		1962	951	10^{-7}	10^{-1}	10^{-10}	10^{-7}	G
39f.	2	3	1.49×10^{-8}		(2001)	(750)	10^{-9}	10^{-1}	10^{-7}	10^{-7}	F LIM
			2.23×10^{-16}		(2001)	(750)	10^{-9}	10^{-1}	10^{-7}	10^{-7}	F LIM
39g.	2	3	1.49×10^{-8}		(2000)	(670)	10^{-9}	10^{-1}	10^{-6}	10^{-7}	F LIM
			2.23×10^{-16}		(2000)	(670)	10^{-9}	10^{-1}	10^{-6}	10^{-7}	F LIM
40a.	3	4	1.49×10^{-8}		13	12	10^{-6}	10^{0}	10^{-11}	10^{-7}	G
			2.23×10^{-16}		13	12	10^{-6}	10^{0}	10^{-11}	10^{-7}	G
40b.	3	4	1.49×10^{-8}		16	10	10^{-6}	10^{0}	10^{-12}	10^{-7}	G
			2.23×10^{-16}		16	10	10^{-6}	10^{0}	10^{-12}	10^{-7}	G
40c.	3	4	1.49×10^{-8}		381	188	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		381	188	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
40d.	3	4	1.49×10^{-8}		2695	1302	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		2695	1302	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
40e.	3	4	1.49×10^{-8}		(3001)	(983)	10^{-7}	10^{0}	10^{-6}	10^{-7}	G
			2.23×10^{-16}		(3001)	(983)	10^{-7}	10^{0}	10^{-6}	10^{-7}	G
40f.	3	4	1.49×10^{-8}		(3003)	(505)	10^{-1}	10^{0}	10^{0}	10^{-2}	F LIM
			2.23×10^{-16}		(3003)	(505)	10^{-1}	10^{0}	10^{0}	10^{-2}	F LIM
40g.	3	4	1.49×10^{-8}		(3002)	(514)	10^{-1}	10^{0}	10^{2}	10^{0}	F LIM
			2.23×10^{-16}		(3002)	(514)	10^{-1}	10^{0}	10^{2}	10^{0}	F LIM
41a.	5	10	1.49×10^{-8}		5	4	10^{-6}	10^{0}	10^{-13}	10^{-7}	G
			2.23×10^{-16}		5	4	10^{-6}	10^{0}	10^{-13}	10^{-7}	G
41b.	5	10	1.49×10^{-8}		6	5	10^{-6}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		6	5	10^{-6}	10^{0}	10^{-10}	10^{-7}	G
41c.	5	10	1.49×10^{-8}		12	11	10^{-6}	10^{0}	10^{-11}	10^{-7}	G
			2.23×10^{-16}		12	11	10^{-6}	10^{0}	10^{-11}	10^{-7}	G
41d.	5	10	1.49×10^{-8}		31	18	10^{-6}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		31	18	10^{-6}	10^{0}	10^{-10}	10^{-7}	G
41e.	5	10	1.49×10^{-8}		154	77	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		154	77	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
41f.	5	10	1.49×10^{-8}		812	368	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		812	368	10^{-7}	10^{0}	10^{-10}	10^{-7}	G
41g.	5	10	1.49×10^{-8}		2137	815	10^{-8}	10^{0}	10^{-10}	10^{-7}	G
			2.23×10^{-16}		2137	815	10^{-8}	10^{0}	10^{-10}	10^{-7}	G

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	n	m	rank tol.	step fac.	f, J evals.	iters.	$\|x^*\|_2$	$\|f^*\|_2$	$\|\bar{g}^*\|_2$	est. err.	conv.
42a.^{0}	4	24	1.49×10^{-8}	0.1	67	38	60.8	10^{-13}	10^{-10}	10^{-25}	x
			2.23×10^{-16}	0.1	67	38	60.8	10^{-13}	10^{-10}	10^{-25}	x
42b.^{0}	4	24	1.49×10^{-8}	0.1	611	316	61.9	10^{-13}	10^{-10}	10^{-25}	x
			2.23×10^{-16}	0.1	(4002)	(1561)	10^5	10^2	10^{11}	10^5	F LIM
42c.^{0}	4	24	1.49×10^{-8}	0.1	33	26	60.3	10^{-13}	10^{-11}	10^{-27}	G, X
			2.23×10^{-16}	0.1	33	26	60.3	10^{-13}	10^{-11}	10^{-27}	G, X
42d.^{0}	4	24	1.49×10^{-8}	0.1	27	23	60.3	10^{-14}	10^{-11}	10^{-28}	G, X
			2.23×10^{-16}	0.1	27	23	60.3	10^{-14}	10^{-11}	10^{-28}	G, X
43a.^{0}	5	16	1.49×10^{-8}	1.0	22	14	54.0	10^{-14}	10^{-11}	10^{-27}	G
			2.23×10^{-16}	1.0	22	14	54.0	10^{-14}	10^{-11}	10^{-27}	G
43b.^{0}	5	16	1.49×10^{-8}	1.0	1167	392	62.1	10^{-1}	10^{-11}	10^{-2}	G
			2.23×10^{-16}	1.0	1167	392	62.1	10^{-1}	10^{-11}	10^{-2}	G
43c.^{0}	5	16	1.49×10^{-8}	1.0	23	14	54.0	10^{-14}	10^{-12}	10^{-28}	G
			2.23×10^{-16}	1.0	23	14	54.0	10^{-14}	10^{-12}	10^{-28}	G
43d.^{0}	5	16	1.49×10^{-8}	1.0	19	9	54.0	10^{-14}	10^{-12}	10^{-27}	G
			2.23×10^{-16}	1.0	19	9	54.0	10^{-14}	10^{-12}	10^{-27}	G
43e.^{0}	5	16	1.49×10^{-8}	1.0	37	19	54.0	10^{-14}	10^{-11}	10^{-27}	G
			2.23×10^{-16}	1.0	37	19	54.0	10^{-14}	10^{-11}	10^{-27}	G
43f.^{0}	5	16	1.49×10^{-8}	2.0	20	11	54.0	10^{-14}	10^{-12}	10^{-27}	G
			2.23×10^{-16}	2.0	20	11	54.0	10^{-14}	10^{-12}	10^{-27}	G
44a.^{0}	6	6	1.49×10^{-8}		125	29	4.06	10^{-14}	10^{-12}	10^{-27}	G
			2.23×10^{-16}		125	29	4.06	10^{-14}	10^{-12}	10^{-27}	G
44b.^{0}	6	6	1.49×10^{-8}		5	4	3.52	10^{-15}	10^{-13}	10^{-29}	ABS F, G
			2.23×10^{-16}		5	4	3.52	10^{-15}	10^{-13}	10^{-29}	ABS F, G
44c.^{0}	6	6	1.49×10^{-8}		52	18	20.6	10^{-14}	10^{-11}	10^{-29}	ABS F
			2.23×10^{-16}		52	18	20.6	10^{-14}	10^{-11}	10^{-29}	ABS F
44d.^{0}	6	6	1.49×10^{-8}		36	15	15.3	10^{-14}	10^{-11}	10^{-29}	ABS F G
			2.23×10^{-16}		36	15	15.3	10^{-14}	10^{-11}	10^{-29}	ABS F G
44e.^{0}	6	6	1.49×10^{-8}		70	23	9.27	10^{-15}	10^{-12}	10^{-29}	ABS F G
			2.23×10^{-16}		70	23	9.27	10^{-15}	10^{-12}	10^{-29}	ABS F G
45a.^{0}	8	8	1.49×10^{-8}		125	29	4.06	10^{-14}	10^{-12}	10^{-27}	G
			2.23×10^{-16}		125	29	4.06	10^{-14}	10^{-12}	10^{-27}	G
45b.^{0}	8	8	1.49×10^{-8}		5	4	3.56	10^{-15}	10^{-13}	10^{-29}	ABS F G
			2.23×10^{-16}		5	4	3.56	10^{-15}	10^{-13}	10^{-29}	ABS F G
45c.^{0}	8	8	1.49×10^{-8}		52	18	20.6	10^{-14}	10^{-11}	10^{-29}	ABS F
			2.23×10^{-16}		52	18	20.6	10^{-14}	10^{-11}	10^{-29}	ABS F
45d.^{0}	8	8	1.49×10^{-8}		36	15	15.3	10^{-15}	10^{-11}	10^{-29}	ABS F G
			2.23×10^{-16}		36	15	15.3	10^{-15}	10^{-11}	10^{-29}	ABS F G
45e.^{0}	8	8	1.49×10^{-8}		70	23	9.31	10^{-14}	10^{-11}	10^{-28}	G
			2.23×10^{-16}		70	23	9.31	10^{-14}	10^{-11}	10^{-28}	G

8.5. Test Problems

Superscripts on problem numbers have the following interpretation :

^{0} : zero-residual problem
^{L} : linear least-squares problem

Problems from Moré, Garbow, and Hillstrom [1981]

	n	m	
1.^{0}	2	2	**Rosenbrock**
2.^{0}	2	2	**Freudenstein and Roth**
3.^{0}	2	2	**Powell Badly Scaled**
4.^{0}	2	3	**Brown Badly Scaled**
5.^{0}	2	3	**Beale**
6.	2	10	**Jennrich and Sampson**
7.^{0}	3	3	**Helical Valley**
8.	3	15	**Bard**
9.	3	15	**Gaussian**
10.	3	16	**Meyer**
11.^{0}	3	10	**Gulf Research and Development**†
12.^{0}	3	10	**Box 3-Dimensional**
13.^{0}	4	4	**Powell Singular**
14.^{0}	4	6	**Wood**
15.	4	11	**Kowalik and Osborne**
16.	4	20	**Brown and Dennis**
17.	5	33	**Osborne 1**
18.^{0}	6	13	**Biggs EXP6**‡

† For the **Gulf Research and Development Function (# 11)**, the formula

$$\phi_i(x) = \exp\left[-\frac{|y_i \; mi \; x_2|^{x_3}}{x_1}\right] - t_i$$

given in Moré, Garbow, and Hillstrom [1981] for the residual functions is in error. The correct formula is

$$\phi_i(x) = \exp\left[-\frac{|y_i - x_2|^{x_3}}{x_1}\right] - t_i$$

(see Moré, Garbow, and Hillstrom [1978]).

‡ For the **Biggs EXP6 Function (# 18)**, the minmum value for the sum of squares is given in Moré, Garbow, and Hillstrom [1981] as $5.65565\ldots \times 10^{-3}$. It can be easily verified that the residuals vanish at several points (for example $(1, 10, 1, 5, 4, 3)$).

Problems from Moré, Garbow, and Hillstrom [1981] (continued)

	n	m	
19.	11	65	**Osborne 2†**
20a.	6	31	**Watson**
20b.	9	31	**Watson**
20c.	12	31	**Watson**
20d.	20	31	**Watson**
21a.^{0}	10	10	**Extended Rosenbrock**
21b.^{0}	20	20	**Extended Rosenbrock**
22a.^{0}	12	12	**Extended Powell Singular**
22b.^{0}	20	20	**Extended Powell Singular**
23a.	4	5	**Penalty I**
23b.	10	11	**Penalty I**
24a.	4	8	**Penalty II**
24b.	10	20	**Penalty II**
25a.^{0}	10	12	**Variably Dimensioned**
25b.^{0}	20	22	**Variably Dimensioned**
26a.^{0}	10	10	**Trigonometric**
26b.^{0}	20	20	**Trigonometric**
27a.^{0}	10	10	**Brown Almost Linear**
27b.^{0}	20	20	**Brown Almost Linear**
28a.^{0}	10	10	**Discrete Boundary Value**
28b.^{0}	20	20	**Discrete Boundary Value**
29a.^{0}	10	10	**Discrete Integral**
29b.^{0}	20	20	**Discrete Integral**
30a.^{0}	10	10	**Broyden Tridiagonal**
30b.^{0}	20	20	**Broyden Tridiagonal**
31a.^{0}	10	10	**Broyden Banded**
31b.^{0}	20	20	**Broyden Banded**
32.^{L}	10	20	**Linear — Full Rank**
33.^{L}	10	20	**Linear — Rank 1**
34.^{L}	10	20	**Linear — Rank 1 with Zero Columns and Rows**
35a.	8	8	**Chebyquad**
35b.^{0}	9	9	**Chebyquad**
35c.	10	10	**Chebyquad**

† For **Osborne's Second Function (# 19)**, the value of $f(x^*)$ is given (to six figures) in Moré, Garbow, and Hillstrom [1981] as 4.01377×10^{-2}. The smallest value we were able to obtain was 4.01683×10^{-2}.

Matrix Square Root Problems

	n	m	
36a.^{0}	4	4	**Matrix Square Root 1**
36b.^{0}	9	9	**Matrix Square Root 2**
36c.^{0}	9	9	**Matrix Square Root 3**
36d.^{0}	9	9	**Matrix Square Root 4**

These test problems come from a private communication of S. Hammarling to P. E. Gill in 1983.

	MATRIX	SQUARE ROOT
36a.^{0}	$\begin{pmatrix} 10^{-4} & 1 \\ 0 & 10^{-4} \end{pmatrix}$	$\begin{pmatrix} 10^{-2} & 50 \\ 0 & 10^{-2} \end{pmatrix}$
36b.^{0}	$\begin{pmatrix} 10^{-4} & 1 & 0 \\ 0 & 10^{-4} & 0 \\ 0 & 0 & 10^{-4} \end{pmatrix}$	$\begin{pmatrix} 10^{-2} & 50 & 0 \\ 0 & 10^{-2} & 0 \\ 0 & 0 & 10^{-2} \end{pmatrix}$
36c.^{0}	$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$
36d.^{0}	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

• The identity matrix was used as the starting value in all instances. Note that the iteration should not be started with the zero matrix because it is a stationary point of the sum of squares.

Problems from Salane [1987]

	n	m	
37.	2	16	**Hanson 1**
38.	3	16	**Hanson 2**

Problems from McKeown [1975a] (also McKeown [1975b])

	n	m		μ
39a.	2	3	**McKeown 1**	0.001
39b.	2	3	**McKeown 1**	0.01
39c.	2	3	**McKeown 1**	0.1
39d.	2	3	**McKeown 1**	1.0
39e.	2	3	**McKeown 1**	10.0
39f.	2	3	**McKeown 1**	100.0
39g.	2	3	**McKeown 1**	1000.0
40a.†	3	4	**McKeown 2**	0.001
40b.†	3	4	**McKeown 2**	0.01
40c.†	3	4	**McKeown 2**	0.1
40d.†	3	4	**McKeown 2**	1.0
40e.†	3	4	**McKeown 2**	10.0
40f.†	3	4	**McKeown 2**	100.0
40g.†	3	4	**McKeown 2**	1000.0
41a.	5	10	**McKeown 3**	*0.001*
41b.	5	10	**McKeown 3**	0.01
41c.	5	10	**McKeown 3**	0.1
41d.	5	10	**McKeown 3**	1.0
41e.	5	10	**McKeown 3**	10.0
41f.	5	10	**McKeown 3**	100.0
41g.	5	10	**McKeown 3**	1000.0

† In the data defining this problem given in McKeown [1975a] and [1975b], the matrix

$$B = \begin{pmatrix} 2.95137 & 4.87407 & -2.0506 \\ 4.87407 & 9.39321 & -3.93181 \\ -2.0506 & -3.93189 & 2.64745 \end{pmatrix}$$

is in error (it should be symmetric). The value

$$B = \begin{pmatrix} 2.95137 & 4.87407 & -2.0506 \\ 4.87407 & 9.39321 & -3.93189 \\ -2.0506 & -3.93189 & 2.64745 \end{pmatrix},$$

which is correct to six decimal digits, was used in our formulation of the problem.

Problems from DeVilliers and Glasser [1981] (also Salane [1987])

	n	m		starting value
42a.^{0}	4	24	**DeVilliers and Glasser 1**	(1.0, 8.0, 4.0, 4.412)
42b.^{0}	4	24	**DeVilliers and Glasser 1**	(1.0, 8.0, 8.0, 1.0)
42c.^{0}	4	24	**DeVilliers and Glasser 1**	(1.0, 8.0, 1.0, 4.412)
42d.^{0}	4	24	**DeVilliers and Glasser 1**	(1.0, 8.0, 4.0, 1.0)
43a.^{0}	5	16	**DeVilliers and Glasser 2**	(45.0, 2.0, 2.5, 1.5, 0.9)
43b.^{0}	5	16	**DeVilliers and Glasser 2**	(42.0, 0.8, 1.4, 1.8, 1.0)
43c.^{0}	5	16	**DeVilliers and Glasser 2**	(45.0, 2.0, 2.1, 2.0, 0.9)
43d.^{0}	5	16	**DeVilliers and Glasser 2**	(45.0, 2.5, 1.7, 1.0, 1.0)
43e.^{0}	5	16	**DeVilliers and Glasser 2**	(35.0, 2.5, 1.7, 1.0, 1.0)
43f.^{0}	5	16	**DeVilliers and Glasser 2**	(42.0, 0.8, 1.8, 3.15, 1.0)

Problems from Dennis, Gay, and Vu [1985]

	n	m		starting value
44a.^{0}†	6	6	**Exp. 791129**	(.299, −0.273, −.474, .474, −.0892, .0892)‡
44b.^{0}†	6	6	**Exp. 791226**	(−.3, .3, −1.2, 2.69, 1.59, −1.5)
44c.^{0}†	6	6	**Exp. 0121a**	(−.041, .03, −2.565, 2.565, −.754, .754)‡
44d.^{0}†	6	6	**Exp. 0121b**	(−.056, .026, −2.991, 2.991, −.568, .568)
44e.^{0}†	6	6	**Exp. 0121c**	(−.074, .013, −3.632, 3.632, −.289, .289)
45a.^{0}	8	8	**Exp. 791129**	(.299, .186, −0.273, .0254, −0.474, −.0892, .0892)‡
45b.^{0}	8	8	**Exp. 791226**	(−.3, −.39, .3, −.344, −1.2, 2.69, 1.59, −1.5)
45c.^{0}	8	8	**Exp. 0121a**	(−.041, −.775, .03, −.047, −2.565, 2.565, −.754, .754)‡
45d.^{0}	8	8	**Exp. 0121b**	(−.056, −.753, .026, −.047, −2.991, 2.991, −.568, .568)
45e.^{0}	8	8	**Exp. 0121c**	(−.074, −.733, .013, −.034, −3.632, 3.632, −.289, .289)

† Variables x_2 and x_4 (b and d in Dennis, Gay, and Vu [1985]) are eliminated from the linear constraints in order to get the 6-variable formulation of the problem (see Dennis, Gay, and Vu [1985]).

‡ Specification of some starting values in Dennis, Gay, and Vu [1985] is incomplete. The correct values were obtained from D. M. Gay in 1986.

9. Bibliography

Al-Baali, M., and R. Fletcher, "Variational Methods for Non-Linear Least Squares", *Journal of the Operational Research Society*, Vol. 36 No. 5 (May 1985) 405–421.

Bard, Y., "Comparison of Gradient Methods for the Solution of Parameter Estimation Problems", SIAM *Journal on Numerical Analysis* Vol. 7 No. 1 (March 1970) 157–186.

Brent, R. P., *Algorithms for Minimization Without Derivatives*, Prentice-Hall (1973).

Dennis, J. E., "III.2 Nonlinear Least Squares and Equations", in *The State of the Art in Numerical Analysis*, D. Jacobs (ed.), Academic Press (1977) 269–312.

Dennis, J. E., and J. J. Moré, "Quasi-Newton Methods : Motivation and Theory", SIAM *Review*, Vol. 19 No. 1 (January 1977) 46–89.

Dennis, J. E., and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall (1983).

Dennis, J. E., D. M. Gay, and P. A. Vu, "A New Nonlinear Equations Test Problem", Technical Report 83-16, Mathematical Sciences Department, Rice University (June 1983 — revised May 1985).

Deuflhard, P., and V. Apostolescu, "A Study of the Gauss-Newton Algorithm for the Solution of Nonlinear Least Squares Problems", in *Special Topics in Applied Mathematics*, North-Holland (1980) 129–150.

DeVilliers, N., and D. Glasser, "A Continuation Method for Nonlinear Regression", SIAM *Journal on Numerical Analysis*, Vol. 18 No. 6 (December 1981) 1139–1154.

Dongarra, J. J., J. R. Bunch, C. B. Moler, and G. W. Stewart, LINPACK *Users' Guide*, SIAM (1979).

Fletcher, R., "Function Minimization Without Evaluating Derivatives — A Review", *Computer Journal* 8 (1963) 163–168.

Fletcher, R., *Practical Methods of Optimization : Volume I, Unconstrained Optimization*, Wiley (1980).

Fraley, C., *Solution of Nonlinear Least-Squares Problems*, Technical Report STAN–CS–87–1165, Ph. D. thesis, Department of Computer Science, Stanford University and Report CLaSSiC–87–04, Center for Large Scale Scientific Computation, Stanford University (July 1987).

Gill, P. E., W. Murray, M. A. Saunders, and M. H. Wright, "Two Steplength Algorithms for Numerical Optimization", Technical Report SOL 79-25, Systems Optimization Laboratory, Department of Operations Research, Stanford University (1979).

Gill, P. E., W. Murray, and M. H. Wright, *Practical Optimization*, Academic Press (1981).

Gill, P. E., S. J. Hammarling, W. Murray, M. A. Saunders, and M. H. Wright, "User's Guide for LSSOL (Version 1.0): A Fortran Package for Constrained Linear Least-Squares and Convex Quadratic Programming", Technical Report SOL 86-1, Systems Optimization Laboratory, Department of Operations Research, Stanford University (January 1986a).

Gill, P. E., W. Murray, M. A. Saunders, and M. H. Wright, "Users Guide for NPSOL (Version 4.0) : A Fortran Package for Nonlinear Programming", Technical Report SOL 86-2, Systems Optimization Laboratory, Department of Operations Research, Stanford University (January 1986b).

Golub, G. H., and C. L. Van Loan, *Matrix Computations*, Johns-Hopkins (1983).

Häussler, W. M., "A Kantorovich-Type Convergence Analysis for the Gauss-Newton Method", *Numerische Mathematik*, Vol. 48 No. 1 (1986) 119–125.

Lawson, C. L., and R. J. Hanson, *Solving Least Squares Problems*, Prentice Hall (1974).

McKeown, J. J., "Specialized versus General-Purpose Algorithms for Minimising Functions that are Sums of Squared Terms", *Mathematical Programming* 9 (1975a) 57–68.

McKeown, J. J., "On Algorithms for Sums of Squares Problems", Paper 14 in *Towards Global Optimization*, L. C. W. Dixon and G. Szegö (eds.), North-Holland (1975b) 229–257.

Moré, J. J., "The Levenberg-Marquardt Algorithm: Implementation and Theory", in *Numerical Analysis — Proceedings Dundee 1977, Lecture Notes in Mathematics*, Vol. 630, Springer-Verlag (1978) 105–116.

Moré, J. J., B. S. Garbow, and K. E. Hillstrom, "Testing Unconstrained Optimization Software", Technical Report TM-324, Applied Mathematics Division, Argonne National Laboratory (July 1978).

Moré, J. J., B. S. Garbow, and K. E. Hillstrom, "Testing Unconstrained Optimization Software", ACM *Transactions on Mathematical Software*, Vol. 7 No. 1 (March 1981) 17–41.

Nocedal, J., and M. L. Overton, "Projected Hessian Updating Algorithms for Nonlinearly Constrained Optimization", SIAM *Journal on Numerical Analysis*, Vol. 22 No. 5 (October 1985).

Osborne, M. R., "Some Aspects of Non-linear Least Squares Calculations", in *Numerical Methods for Nonlinear Optimization*, F. A. Lootsma (ed.), Academic Press (1972) 171–189.

Powell, M. J. D., "A Hybrid Method for Nonlinear Equations", in *Numerical Methods for Nonlinear Algebraic Equations*, P. Rabinowitz (ed.), Gordon and Breach (1970a) 87–114.

Ramsin, H., and P-Å. Wedin, "A Comparison of some Algorithms for the Nonlinear Least Squares Problem", *BIT* 17 No. 1 (1977) 72–90.

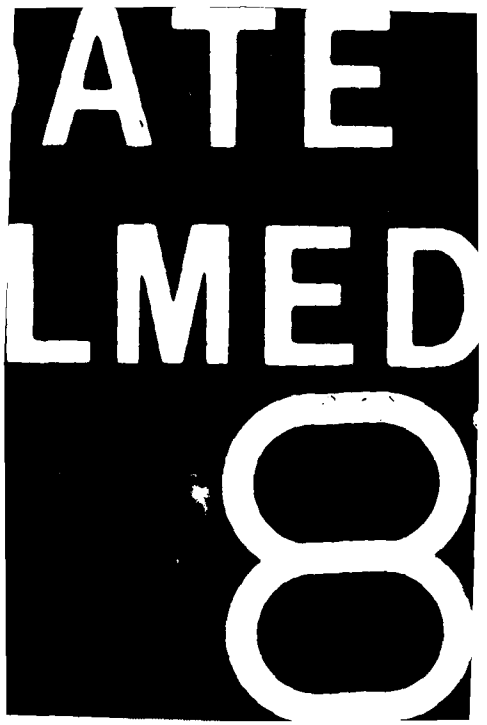
Ruhe, A., "Accelerated Gauss-Newton Algorithms for Nonlinear Least Squares Problems", *BIT*, Vol. 19 (1979) 356–367.

Salane, D. E., "A Continuation Approach for Solving Large Residual Nonlinear Least Squares Problems", SIAM *Journal on Scientific and Statistical Computing*, Vol. 8 No. 4 (July 1987) 655-669.

Schaback, R., "Convergence Analysis of the General Gauss-Newton Algorithm", *Numerische Mathematik*, Vol. 46 No. 2 (1985) 281–309.

Stewart, G. W., *Introduction to Matrix Computations*, Academic Press (1973).

Wedin, P.-Å., and P. Lindström, "Methods and Software for Nonlinear Least Squares Problems", Report UMINF-133.87, ISSN-0348-0542, University of Umeå, Institute of Information Processing (May 1987).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