Theoretical and Computational Aspects of Nonlinear Regression

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ABSTRACT

Nonlinear regression problems can often be stated in the form: minimize $\|y - f(\theta)\|^2$, where y is a fixed n-vector of observations and f is a nonlinear mapping from E^r to E^n. Such problems constitute an important class of nonlinear unconstrained minimization problems. Theoretical and computational aspects of some numerical method for nonlinear regression are described with emphasis on the relationship to mathematical programming.

1. Introduction

The nonlinear regression problem to be dealt with is conveniently stated in the form,

$$\underset{\theta}{\text{minimize}} \; \|y - f(\theta)\|^2 , \qquad (1.1)$$

where y is a fixed n-vector of "observations", f is a continuously differentiable nonlinear mapping from E^p to E^n, θ is the vector variable (the "parameters") in E^p, and the norm is the Euclidean norm in E^n. (In engineering and statistical work, it is customary to write $g(X_k, \theta)$ in place of $f_k(\theta)$ $(k = 1, \ldots, n)$, where g is a mapping (the "model") from E^{m+p} to E^1 and X_k is the setting of the independent variables at the k^{th} "experiment". In this analysis of nonlinear regression, however, references to the function $g(X, \theta)$ and the values X_k would tend to complicate and unnecessarily restrict the scope of the presentation.) Theoretical and computational aspects of iterative techniques for solving nonlinear regression problems will be discussed in this paper. Section 2 contains a description of some previously developed techniques, starting with a procedure proposed by Gauss [1], and introduces a new method, the Modified Damped Least Squares (MDLS) algorithm, devised by the author. Some numerical aspects and convergence properties of MDLS are proved in Section 3, and compared with those of other methods. Section 4 deals with computational devices that have been found in practice to improve the efficiency and the reliability of MDLS. Finally, an evaluation of numerical results for several difficult problems is given in Section 5.

Some of the notation and notational conventions to be used throughout the paper will be now described. With the exception of gradients, which are always taken to be row vectors, all vectors without the superscript ^{T}(denoting transpose) will be column vectors. Hence we may write the nonlinear regression problem (1.1) as

$$\underset{\theta}{\text{minimize}} \quad (f(\theta) - y)^T(f(\theta) - y) . \tag{1.2}$$

For notational purposes it is convenient to define the vector error function and the sum of squared errors function:

$$e(\theta) \equiv f(\theta) - y \tag{1.3}$$

$$s(\theta) \equiv e^T(\theta)e(\theta) = \|y - f(\theta)\|^2 . \tag{1.4}$$

It is easily verified that the gradient of $s(\theta)$, to be denoted by $s'(\theta)$ (a row vector) is given by

$$s'(\theta) = 2e^T(\theta)f'(\theta) , \tag{1.5}$$

where $f'(\theta)$ is the $n \times p$ Jacobian matrix $(\partial f_i(\theta)/\partial \theta_j)$. By differentiating (1.5) we obtain the $p \times p$ Hessian matrix of second partials of $s(\theta)$,

$$s''(\theta) \equiv 2f'(\theta)^T f'(\theta) + 2e^T(\theta)f''(\theta) , \tag{1.6}$$

where

$e^T(\theta)f''(\theta)$ denotes the summation

$$\sum_{\ell=1}^{n} e_\ell(\theta)f_\ell''(\theta) . \tag{1.7}$$

(Note that the expression $e^T(\theta)f''(\theta)$ is merely a symbolic representation for the matrix given by (1.7). Dimensionally the expression makes no sense when n and p are greater than 1.)

2. Iterative Methods for Nonlinear Regression

Since nonlinear regression problems form a class of unconstrained minimization problems, it is natural to seek iterative methods for their solution that take advantage of their particular structure. The first such method appears to have been described by Gauss [1] in 1809. (All of the methods to be presented in this section are iterative algorithms that assume that an initial guess θ^o for the parameters is given. Hence, for each method we will simply describe the basic iterative procedure that is used to derive the $(i+1)^{st}$ iterate, θ^{i+1}, from the i^{th} iterate, θ^i. Given an initial guess θ^o, a sequence $\theta^1, \theta^2, \ldots$ of iterates can thus, in theory, be derived. The convergence properties of these sequences are derived in the next section of the paper.) An iteration of the Gauss-Newton method, as it is usually referred to, essentially consists of linearizing <u>within</u> the norm signs of (1.1), and solving the resulting linear least squares problem.

Gauss-Newton Method

1) Determine the solution of the linear least squares problem:

$$\underset{\Delta}{\text{minimize}} \ \|f(\theta^i) + f'(\theta^i)\Delta - y\|^2 \tag{2.1}$$

2) Let $\theta^{i+1} = \theta^i + \Delta^*$, where Δ^* is the solution of (2.1).
(Assuming that the matrix

$$F \equiv f'(\theta^i)^T f'(\theta^i) \tag{2.2}$$

is nonsingular, the solution of (2.1) is given by

$$\Delta^* = -F^{-1}(f'(\theta^i)^T e(\theta^i)) \tag{2.3}$$

This is the usual assumption in the Gauss-Newton method; the procedure may be directly extended to the case in which F is singular by using the generalized inverse of $f'(\theta^i)$ as suggested by Ben-Israel [2].) Note that this reduces to Newton's method when $p = n$, since in such a case nonsingularity of F implies $F^{-1} = (f'(\theta^i))^{-1}(f'(\theta^i)^T)^{-1}$ and thus $\Delta^* = -(f'(\theta^i))^{-1}e(\theta^i)$, the correction of Newton's method.

As might be expected, the solution Δ^* of (2.1) will in general <u>not</u> satisfy the monotonicity or "stability" property

$$s(\theta^i + \Delta^*) < s(\theta^i) . \tag{2.4}$$

Consequently, convergence of the Gauss-Newton iterates to a stationary point will not occur unless the initial guess θ^o is, in some sense, "good". Pereyra [3] and Ben-Israel [2] have stated sufficient conditions on θ^o that guarantee convergence to a stationary point. These conditions will be discussed in the next section.

The Gauss-Newton method persisted as one of the standard methods for the solution of nonlinear regression problems until 1944 when Levenberg [4] developed the method of Damped Least Squares (DLS) in order to obtain better convergence properties. An iteration of DLS is based on the solution of problems of the form

$$\underset{\Delta}{\text{minimize}} \quad \|f(\theta^i) + f'(\theta^i)\Delta - y\|^2 + \lambda\Delta^T W\Delta , \qquad (2.5)$$

where λ is a non-negative scalar (the <u>damping factor</u>) and W is a positive definite diagonal matrix. The term $\lambda\Delta^T W\Delta$ has the effect of "damping" the size of the solution of the unconstrained problem. For $\lambda > 0$ the problem (2.5) (without any assumptions on F) will have the unique solution $\Delta^*(\lambda, W)$ given by the formula

$$\Delta^*(\lambda, W) = -(F + \lambda W)^{-1}(f'(\theta^i)^T e(\theta^i)) . \qquad (2.6)$$

Damped Least Squares (DLS) Method

1) Solve problems of the form (2.5) for increasing values of the damping factor λ until a value λ_i^* is determined for which $s(\theta^i + \Delta^*(\lambda_i^*, W))$ is an "approximate minimum" of $s(\theta^i + \Delta^*(\lambda, W))$ considered as a function of λ.

2) Let $\theta^{i+1} = \theta^i + \Delta^*(\lambda_i^*, W)$.

The procedures by which an "approximate minimum" is determined in DLS and in the two remaining methods of this section will be described in detail in sections 3 and 4. Here we shall point out only that Levenberg showed that for any positive definite diagonal matrix W, the inequality

$$s(\theta^i + \Delta^*(\lambda, W)) < s(\theta^i) \qquad (2.7)$$

is satisfied for all sufficiently large λ, so that one of the criteria for λ_i^* is that (2.7) be satisfied when $\lambda = \lambda_i^*$. Note, however, that if the initial guess for λ_i^* does not satisfy (2.7), then the modified least squares problem (2.5) must be solved with successively larger values of λ until monotonicity is achieved.

In 1961, Hartley [5] described an approach to stability based upon a one-dimensional search in the direction of Δ^*, the solution of (2.1).

Hartley's Method

1) Determine the solution Δ^* of the linear least squares problem (2.1).

2) Determine a <u>step-length factor</u> γ_i^* such that $s(\theta^i + \gamma_i^* \Delta^*)$ is an "approximate minimum" of $s(\theta^i + \gamma\Delta^*)$ for $\gamma \geq 0$.

3) Let $\theta^{i+1} = \theta^i + \gamma_i^* \Delta^*$

It is easily shown that if $s'(\theta^i) \neq 0$, then $s'(\theta^i)\Delta^* < 0$ and consequently for all sufficiently small step-length factors we have

$$s(\theta^i + \gamma\Delta^*) < s(\theta^i) . \tag{2.8}$$

Hence, Hartley's method also (in theory) leads to a set of monotone decreasing function values, but the solution of only one least squares problem ((2.1)) is required at each iteration.

The modified Damped Least Squares (MDLS) method to be described below extends the DLS method in a manner analogous to Hartley's extension of the Gauss-Newton method. In MDLS the matrix of weights W for the i^{th} iteration is taken to be the diagonal matrix D whose diagonal elements are those of the matrix F. The diagonal entries of D are all positive unless one or more columns of $f'(\theta^i)$ are identically 0, hence the underlying assumption of MDLS is that no such column vanishes. (This is one of two suggestions for W advanced by Levenberg. The other called for setting $W = I$, the identity matrix. The DLS method in the case $W = D$ is often referred to in the literature as <u>Marquardt's method</u>. Levenberg's original paper apparently received very little attention, and it was not until after DLS was rediscovered by Marquart [6] that the use of the procedure became widespread.) Note that adding the matrix λD to F is equivalent to multiplying the diagonal elements of F by the factor $(1 + \lambda)$.

Modified Damped Least Squares (MDLS) Method

1) Choose a damping factor λ_i

2) Determine the solution $\Delta^*(\lambda_i, D)$ of the corresponding damped least squares problem.

3) Determine a step-length factor $\overline{\gamma}_i$ such that $s(\theta^i + \overline{\gamma}_i \cdot \Delta^*(\lambda_i, D))$ is an "approximate minimum" of $s(\theta^i + \gamma\Delta^*(\lambda_i, D))$ for $\gamma \geq 0$.

4) Let $\theta^{i+1} = \theta^i + \overline{\gamma}_i\Delta^*(\lambda_i, D)$.

Of course, if λ_i is taken to be 0 for all i the iterative procedure reduces to Hartley's method. It will be shown in the next section that $s'(\theta^i) \neq 0$ implies that $s'(\theta^i)\Delta^*(\lambda, W) < 0$ for any positive definite matrix W and any $\lambda \geq 0$. Hence the iterates of MDLS will have the property that

$$s(\theta^{i+1}) < s(\theta^i) \tag{2.9}$$

unless θ^i is a stationary point of $s(\theta)$. The algorithm by which λ_i is chosen at the i^{th} iteration will be described in section 4.

3. Theoretical Comparison

In this section we shall derive some theoretical properties of the methods to use as the basis for further comparison. The following three properties of the problem (2.5) are obtained under the assumptions that D is positive definite and that $W = D$.

a) If $s'(\theta^i) \neq 0$, then for $\lambda > 0$

$$s'(\theta^i)\Delta^*(\lambda, D) < 0 , \tag{3.1}$$

where $$\Delta^*(\lambda, D) = -(F + \lambda D)^{-1}(f'(\theta^i)^T e(\theta^i)) . \tag{3.2}$$

b) For all $\lambda > 0$, $\Delta^*(\lambda, D)$ is the unique solution of (2.5).

c) The condition number (here taken to be the ratio of the maximum over the minimum eigenvalue) of $F + \lambda D$ is a nonincreasing function of λ.

The proof of a) follows easily from the facts that $(F + \lambda D)^{-1}$ is positive definite for $\lambda > 0$ and that by using the equation (1.5) for the gradient of $s(\theta)$ we have

$$\Delta^*(\lambda, D) = -(1/2)(F + \lambda D)^{-1} s'(\theta^i)^T \tag{3.3}$$

To prove property b) note that $F = f'(\theta^i)^T f'(\theta^i)$ is either positive semi-definite or positive definite, so that $F + \lambda D$ is positive definite and hence nonsingular for $\lambda > 0$. By setting $W = D$ and taking the gradient with respect to Δ in (2.5), it is easily verified that the unique solution is given by (3.2). If F^{-1} exists, then (3.2) is also valid for $\lambda = 0$ and reduces to the formula for Δ^* in this case. Note that it is not necessary to assume nonsingularity of F when $\lambda > 0$, so that MDLS can be applied in some cases in which Hartley's method cannot. Even when F^{-1} does exist, the use of a positive damping factor improves the conditioning of the system of equations that must be solved, as asserted in property c). In order to demonstrate this fact denote the maximum eigenvalues of D and $F + \lambda D$ by d_1 and $\alpha_1(\lambda)$ respectively, and the minimum eigenvalues of D and $F+\lambda D$ by d_p and $\alpha_p(\lambda)$ respectively. If $\lambda'' > \lambda' \geq 0$, then the following inequalities result from applying the theorem that the field of values of a normal matrix is the convex hull of the spectrum:

$$\begin{aligned}\frac{\alpha_1(\lambda'')}{\alpha_p(\lambda'')} &\leq \frac{\alpha_1(\lambda') + (\lambda'' - \lambda')d_1}{\alpha_p(\lambda') + (\lambda'' - \lambda')d_p} \\ &\leq \frac{\alpha_1(\lambda') + (\lambda'' - \lambda')(1 + \lambda')^{-1}\alpha_1(\lambda')}{\alpha_p(\lambda') + (\lambda'' - \lambda')(1 + \lambda')^{-1}\alpha_p(\lambda')} \\ &= \frac{\alpha_1(\lambda')}{\alpha_p(\lambda')}\end{aligned}$$

Let us now compare the methods of the previous section in the light of properties a) - c) . It has already been observed that the original Gauss-Newton method can be guaranteed to converge only when the starting point θ^o is sufficiently close to a stationary point. Because of the monotonicity property of the other three methods (in the case of MDLS, (3.1) guarantees monotonicity), they are, under rather weak assumptions, globally convergent. That is, regardless of the starting point, they will converge to a stationary point of the original problem if a stationary point exists. This idea will be made precise later in this section. DLS has the disadvantage that an evaluation of the effect of different damping factors at each iteration is inefficient (relative to Hartley's method or MDLS) because a number of systems of equations (instead of just one) must be solved. Lastly, according to properties b) and c), the case in which the matrix F is singular or ill-conditioned is readily handled in MDLS, but not in Hartley's method.

In order to establish the convergence properties of MDLS, it is necessary to rigorously define what is meant by an "approximate minimum" of the one-dimensional search performed at each iteration. One approach to the definition is to require a certain fixed percentage $\beta \in (0, 1)$ of "optimality" at each iteration. That is, $\overline{\gamma}_i$ is taken to be the first integer power of $1/2$ for which the following inequality is satisfied:

$$s(\theta^i + \overline{\gamma}_i\Delta^*(\lambda_i, D)) \leq s(\theta^i) + \beta \cdot \overline{\gamma}_i \cdot s'(\theta^i)\Delta^*(\lambda_i, D) \tag{3.4}$$

We shall now prove that a $\overline{\gamma}_i$ satisfying (3.4) does indeed exist. If $s'(\theta^i) = 0$, then $\Delta^*(\lambda_i, D) = 0$ and the inequality is trivially satisfied, so assume $s'(\theta^i) \neq 0$. Differentiability of $s(\theta)$ at θ^i implies

$$s(\theta^i + \gamma\Delta) \leq s(\theta^i) + \gamma s'(\theta^i)\Delta + \epsilon(\|\gamma\Delta\|)\|\gamma\Delta\| , \tag{3.5}$$

for all γ and Δ, where $\epsilon(x) \to 0$ as $x \to 0$. In particular, when Δ is taken to be $\Delta^*(\lambda_i, D)$ and γ is sufficiently small,

$$\epsilon(\|\gamma\Delta^*(\lambda_i, D)\|) \leq -(1-\beta)s'(\theta^i)\Delta^*(\lambda_i, D)\|\Delta^*(\lambda_i, D)\|^{-1}.$$

Substituting the latter inequality in (3.5) and replacing γ by $\bar{\gamma}_i$ and Δ by $\Delta^*(\lambda_i, D)$, we obtain (3.4). (Note that when β is chosen very close to 0 the inequality (3.4) is almost equivalent to

$$s(\theta^i + \bar{\gamma}_i\Delta^*(\lambda_i, D)) < s(\theta^i) . \tag{3.6}$$

In fact, from a computational standpoint, since only a finite number of iterations can be performed, the satisfaction of (3.6) for the iterates actually obtained implies the existence of a range of values of β for which the iterates obtained would also satisfy (3.4). However, the inequality (3.6) by itself is not strong enough to guarantee the desired theoretical convergence properties.)

Theorem 1: Let $\{\theta^i\}$ be a sequence of iterates generated by MDLS using the rule given above for the selection of the step-length factor at the i^{th} iteration. If there exists a subsequence $\{\theta^{n_i}\}$ converging to some set of parameters θ^* and if the corresponding subsequence $\{f'(\theta^{n_i})^T f'(\theta^{n_i}) + \lambda_{n_i} D_{n_i}\}$ converges to some positive definite matrix P (D_{n_i} denotes the diagonal matrix whose diagonal coincides with that of $f'(\theta^{n_i})^T f'(\theta^{n_i})$), then $s'(\theta^*) = 0$.

Proof: We will assume that $s'(\theta^*) \neq 0$ and show that this leads to a contradiction. Let $\Delta^{n_i} = -(f'(\theta^{n_i})^T f'(\theta^{n_i}) + \lambda_{n_i} D_{n_i})^{-1}(f'(\theta^{n_i})^T e(\theta^{n_i}))$ and $\Delta^{**} = \lim \Delta^{n_i} = -P^{-1}(f'(\theta^*)^T e(\theta^*))$. Since $s'(\theta^*)$ is assumed not to vanish and P is positive definite, $s'(\theta^*)\Delta^{**} < 0$. Let γ^{**} be the smallest power of $1/2$ satisfying

$$s(\theta^* + \gamma^{**}\Delta^{**}) < s(\theta^*) + \beta \cdot \gamma^{**} \cdot s'(\theta^*)\Delta^{**} .$$

By continuity it follows that for n_i sufficiently large we also have

$$s(\theta^{n_i} + \gamma^{**}\Delta^{n_i}) < s(\theta^{n_i}) + \beta \cdot \gamma^{**} \cdot s'(\theta^{n_i})\Delta^{n_i} ,$$

from which we conclude that

$$s(\theta^{n_i+1}) = s(\theta^{n_i} + \bar{\gamma}_{n_i}\Delta^{n_i}) < s(\theta^{n_i}) + \beta \cdot \gamma^{**} \cdot s'(\theta^{n_i})\Delta^{n_i} .$$

By the monotonicity property (2.9) it follows that $\lim s(\theta^{n_i+1}) = \lim s(\theta^{n_i}) = s(\theta^*)$. Hence, taking limits on both sides of the last inequality yields $s(\theta^*) \leq s(\theta^*) + \beta \cdot \gamma^{**} \cdot s'(\theta^*)\Delta^{**}$, which is impossible since $\beta \cdot \gamma^{**} \cdot s'(\theta^*)\Delta^{**} < 0$.

There are a number of ways of guaranteeing that there will be a convergent subsequence of iterates. One of the simplest is to assume that for any $\bar{\theta} \in E^p$ the set $L(\bar{\theta}) \equiv \{\theta \mid s(\theta) < s(\bar{\theta})\}$ is compact. This hypothesis implies that for an arbitrary starting point θ^o the sequence generated by MDLS will lie in a compact set. The next theorem states that the addition of two further hypotheses leads to convergence of the whole sequence to a stationary point.

<u>Theorem 2:</u> If (a) $L(\bar{\theta})$ is compact for each $\bar{\theta} \in E^p$, (b) $s(\theta)$ has at most a finite number of stationary points having any given function value, (c) $f'(\theta)^T f'(\theta)$ is positive definite for all θ, and (d) there is an upper bound on the damping factor to be used at any iteration, then, given an aribtrary starting point θ^o, the iterates $\{\theta^i\}$ generated by MDLS will converge to a stationary point of $s(\theta)$.

<u>Proof:</u> It follows from hypothesis (a) and the monotonicity of the function values of the iterates that $\{\theta^i\}$

lies in a compact set. Hypotheses (c) and (d) imply by theorem 1 that every accumulation point of $\{\theta^i\}$ will be a stationary point of $s(\theta)$, and (b) implies that there can only be a finite number of these accumulation points, since they must all have the same function value. Using the formula (3.3) and hypotheses (c) and (d), it is easily shown that $\Delta^*(\lambda_i, D) \to 0$. Suppose that the sequence $\{\theta^i\}$ has more than one accumulation point, and let ϵ^* be the minimum distance between any two accumulation points. Since $\{\theta^i\}$ lies in a compact set, there exists an integer N such that for all $i \geq N$ θ^i lies within a ball of radius $\epsilon^*/4$ about some accumulation point. On the other hand, there exists an $N' \geq N$ such that $\|\Delta^*(\lambda_i, D)\| < \epsilon^*/4$ for $i \geq N'$. Hence, for $i \geq N'$ all θ^i must lie within a ball of radius $\epsilon^*/4$ about one particular accumulation point, contradicting the assumed existence of more than one accumulation point.

Note that theorem 2 is a global convergence result that applies to Hartley's method (by setting the upper bound on the damping factor to 0) as well as MDLS. A similar convergence result could also be obtained for DLS if the rule for the selection of the quasi-optimal damping factor at each iteration was analogous to the rule given for $\bar{\gamma}_i$. Recall that the Gauss-Newton method does not have this type of global convergence property.

It is clear from the expression (1.6) for the second derivative $s''(\theta)$ that the sum of squared errors function $s(\theta)$ will in general be non-convex. Hence there is no guarantee that a stationary point located by MDLS (or any other algorithm considered in this paper) will be the global solution of the problem of minimizing $s(\theta)$. The following theorem deals with the rate of convergence to stationary points that will at least be "local minima." Since the theorem below assumes that $\lambda_i \to 0$ (as is usually the case in MDLS), the same convergence rate estimate applies to all of the methods described in section 2 even though it is stated for MDLS.

Theorem 3: Let $\{\theta^i\}$ be a sequence generated by MDLS which converges to a point θ^*. Let m be the minimum eigenvalue of $f'(\theta^*)^T f'(\theta^*)$ and M be the maximum of the absolute values of the eigenvalues of $e^T(\theta^*)f''(\theta^*)$. If $r \equiv M/m < 1$, $\beta < (1-r)/2$, and $\lambda_i \to 0$, then $\overline{\gamma}_i = 1$ for all sufficiently large i and $\limsup \|\theta^{i+1} - \theta^*\| / \|\theta^i - \theta^*\| \leq r$. Moreover, $s(\theta^*)$ will be an isolated local minimum of the function $s(\theta)$.

Proof: (For notational convenience in this proof Δ will be used to denote $\Delta^*(\lambda_i, D)$.) A second-order approximation of the change of function value is given by the equation

$$s(\theta^i + \Delta) - s(\theta^i) = s'(\theta^i)\Delta + 1/2\, \Delta^T s''(\overline{\theta})\Delta \,, \qquad (3.7)$$

where $\overline{\theta} = \theta^i + \delta\Delta$, $\delta \in (0, 1)$. In order to have $\overline{\gamma}_i = 1$, the following inequality is required:

$$\beta \cdot s'(\theta^i)\Delta - (s(\theta^i + \Delta) - s(\theta^i)) \geq 0 \qquad (3.8)$$

Using the relations $s'(\theta^i) = -\Delta^T(2F + 2\lambda_i D)$ and (3.7), the expression on the LHS of the inequality takes the form

$$(1 - \beta)\Delta^T(2F + 2\lambda_i D)\Delta - 1/2\Delta^T s''(\overline{\theta})\Delta =$$

$$\Delta^T[2 \cdot (1 - \beta)F - 1/2 s''(\theta^i) + 2 \cdot (1 - \beta)\lambda_i D -$$

$$1/2(s''(\overline{\theta}) - s''(\theta^i))]\Delta =$$

$$\Delta^T[(1 - 2\beta)F - e^T(\theta^i)f''(\theta^i) + G_i]\Delta \,,$$

where $G_i = 2 \cdot (1 - \beta)\lambda_i D - 1/2(s''(\overline{\theta}) - s''(\theta^i))$.

Since $G_i \to 0$, in order to verify (3.8) for large i, it is necessary only to prove that $(1 - 2\beta)F - e^T(\theta^i)f''(\theta^i)$ converges to a positive definite matrix. But the minimum eigenvalue of

$$(1 - 2\beta)f'(\theta^*)^T f'(\theta^*) - e^T(\theta^*)f''(\theta^*)$$

is bounded from below by the value $(1 - 2\beta)m - M = m(1 - 2\beta - r)$, which is positive under the assumption $\beta < (1 - r)/2$.

To prove the estimate on the rate of convergence note that for large i

$$\theta^{i+1} - \theta^* = \theta^i - \theta^* - 1/2(F + \lambda_i D)^{-1} s'(\theta^i)^T$$

$$= \theta^i - \theta^* - 1/2(F + \lambda_i D)^{-1}[s''(\theta^i)(\theta^i - \theta^*)$$

$$+ s'(\theta^i)^T + s''(\theta^i)(\theta^* - \theta^i)]$$

$$= -1/2(F + \lambda_i D)^{-1}[2e^T(\theta^i)f''(\theta^i)(\theta^i - \theta^*)$$

$$- 2\lambda_i D(\theta^i - \theta^*) + s'(\theta^i)^T + s''(\theta^i)(\theta^* - \theta^i)] .$$

Taking norms on both sides yields

$$\|\theta^{i+1} - \theta^*\| \leq 1/2\|F^{-1}\|[2\|e^T(\theta^i)f''(\theta^i)\| \; \|\theta^i - \theta^*\|$$

$$+ 2\lambda_i \|D\| \; \|\theta^i - \theta^*\| + \|s'(\theta^i)^T + s''(\theta^i)(\theta^* - \theta^i)\|]$$

Since

$$\|s'(\theta^i)^T + s''(\theta^i)(\theta^* - \theta^i)\| = \|s'(\theta^i)^T +$$

$$+ s''(\theta^i)(\theta^* - \theta^i) - s'(\theta^*)^T\| \leq \epsilon_i \|\theta^* - \theta^i\| ,$$

where $\epsilon_i \to 0$, dividing through by $\|\theta^i - \theta^*\|$ yields

$$\|\theta^{i+1} - \theta^*\| / \|\theta^i - \theta^*\| \leq \|F^{-1}\| [\, \|e^T(\theta^i) f''(\theta^i)\|$$

$$+ \lambda_i \|D\| + 1/2\epsilon_i]$$

From which it follows immediately that $\limsup \|\theta^{i+1} - \theta^*\| / \|\theta^i - \theta^*\| \leq m^{-1}M = r$.

Since $s'(\theta^*) = 0$, the final conclusion of the theorem is equivalent to the demonstration that $s''(\theta^*)$ is positive definite. The matrix $s''(\theta^*)$ is positive definite since it is the sum

$$2f'(\theta^*)^T f'(\theta^*) + 2e^T(\theta^*) f''(\theta^*),$$

whose minimum eigenvalue is bounded from below by $m - M > 0$.

As noted previously, both Pereyra and Ben-Israel have also derived convergence results for the Gauss-Newton method. These, however, are sufficient conditions for convergence rather than global convergence results such as theorem 2. In addition, the estimated rates of convergence given by Pereyra and Ben-Israel involve upper bounds on first and second derivatives in a sphere about the initial guess, θ^o. The convergence rate estimate of theorem 3 is more closely related to a result of Daniel [7] for Newton-like methods.

From a qualitative standpoint, theorem 3 indicates that the efficiency of the algorithms of section 2 is related to the magnitude of the error, $e(\theta^*)$, at the stationary point to which the iterates converge. In particular, if $e(\theta^*) = 0$, then $M = 0$ and therefore $r = 0$, so that the rate of convergence is superlinear. This is not surprising, since $e(\theta^*) = 0$ implies (in the context of theorem 3) that $f'(\theta^i)^T f'(\theta^i) \to s''(\theta^*)$, so that the search directions $\Delta^*(\lambda_i, D)$ are a good approximation to the corrections $-s''(\theta^i)^{-1} s'(\theta^i)^T$

of Newton's method for determining a zero of $s'(\theta)$. In this instance, the limiting behavior is similar in principle to the well-known Davidon-Fletcher-Powell method [8] and other quasi-Newton methods that generate matrices that converge to the Hessian matrix (or its inverse) in the limit. In the quasi-Newton methods the approximation to the Hessian is constructed using information from previous iterations, whereas algorithms derived from the Gauss-Newton method take advantage of the special form of the problem to construct an approximation to the Hessian based only on first derivatives at the most recent set of parameter values. Since the reliance of the quasi-Newton methods upon information from previous iterations has been observed to lead to numerical difficulties in some cases [9], the Gauss-Newton approach appears to be preferable in nonlinear regression problems in which a good "fit" of the data is expected. Results of numerical experiments by Pitha and Jones [10] and Bard [11] agree with this conclusion.

4. Computational Devices

Computational experience with certain difficult problems revealed numerical difficulties in applying the MDLS method as outlined in section 2. In order to resolve these difficulties, various computational safeguards were added to the computer program implementing MDLS. This section describes the most important of these safeguards, as well as certain devices introduced to increase efficiency.

a) The program user has the option of introducing <u>explicit</u> bounds on the components of the correction $\theta^{i+1} - \theta^i$ in addition to the <u>implicit</u> bounds resulting from the damping term. (The size of the correction cannot be accurately controlled by damping alone.)

b) One or more univariate searches are performed in the event that numerical difficulties prevent the satisfaction of (3.6). A number of other "alternate" search direction schemes for this type of emergency have also been tested and found to be successful. A further extension of this concept would be to establish at each iteration a set of directions along which searches would be performed until a set of criteria specified by the user were satisfied. In a time-sharing system, the user would even be allowed to establish the order in which directions were tried at each iteration and to exercise his own judgement on the acceptability of the result of a search.

c) The initial damping factor, λ_0, is set to some nominal value such as 1/100 or 1/1000. At the i^{th} iteration, λ_i is set to $4\lambda_i$ if a univariate search was required to reduce the sum of squares function at the $(i-1)^{st}$ iteration; otherwise λ_i is set to $\lambda_{i-1}/4$. This is similar to the rule proposed by Marquardt. Note that if the basic MDLS method as described in section 2 is successful in reducing the sum of squares at each iteration, then $\lambda_i \to 0$.

d) In order to improve efficiency, the method of determining $\overline{\gamma}_i$ presently being used in the program is a modified quadratic interpolation scheme. A number of similar schemes are described by Bard [11].

5. Computational Experience

The computer program implementing MDLS has been successfully tested on a large number of problems and is presently being used on a "production" basis. In this section some representative computational results will be presented.

Rosenbrock's Problem

This is a two variable test problem originally discussed by Rosenbrock [12] and now frequently cited in the literature. In the notation of section 1, the problem is given by $y_1 = y_2 = 0$, $f_1(\theta) = (\theta_2 - \theta_1^2)$, and $f_2 = 0.1(1-\theta_1)$, so that $s(\theta) = (\theta_2 - \theta_1^2)^2 + 0.01(1 - \theta_1)^2$. The starting point is given by $\theta^o = (-1.2, 1.0)$, and the iterates are forced to "track" along a steep-sided parabolic valley to the solution $\theta = (1, 1)$. The solution was obtained in 17 iterations (with a total of 31 function evaluations) by MDLS, in 17 iterations (with a total of 32 function evaluations) by Hartley's method, and in 38 iterations (with a total of 61 function evaluations) by DLS. The performance of the former two methods compares favorably with that of the Fletcher-Powell method as cited in [8]. The Fletcher-Powell method required 18 iterations to obtain a solution, but the more accurate unidirectional searches required in the Fletcher-Powell method imply that the total number of function evaluations in 18 iterations would be much greater than 31.

Thermistor Problem

The data for this problem were furnished to us by J. H. Badley of Shell Development Company. They represent the resistance of a thermistor as a function of temperature.

y	T
34,780	50
28,610	55
23,650	60
19,630	65
16,370	70
13,720	75
11,540	80
9,744	85
8,261	90
7,030	95
6,005	100
5,147	105
4,427	110
3,820	115
3,307	120
2,872	125

The model is given by $f_j(\theta) = \theta_1 \cdot \exp \theta_2/(T_j + \theta_3)$, and the initial values used were $\theta_1^0 = 0.02$, $\theta_2^0 = 4{,}000$, and $\theta_3^0 = 250$.

This problem is of interest because it was the only one tested in which MDLS failed to obtain in 51 iterations a solution when started with a non-zero damping factor. When the damping factor was set initially to 0 (yielding

Hartley's method), however, convergence in 7 iterations to the optimal solution, $\theta_1^* = 0.005609$, $\theta_2^* = 6,181$, $\theta_3^* = 345.2$ was obtained. DLS also failed on this problem.

Spectroscopic Data Problem Set

This is a set of 11 representative problems assembled by D. D. Tunnicliff of Shell Development Company. Each problem in the set involves the fitting of spectrographic data by a sum of nonlinear functions. The simplest function used in the fit has the form

$$\sigma \cdot \exp - [(x - \mu)/\omega]^2 ,$$

where σ, μ, and ω are parameters and x is the independent variable. The performances of Hartley's method and MDLS on this problem set were essentially the same except for the most difficult problem in the set, which involved 35 parameters. On this problem Hartley's method failed to converge to the optimal set of parameters, whereas the iterates of MDLS did converge to the correct values. When applied to this problem set, the DLS method failed on the most difficult problem, as well as two others in the set. Quasi-Newton methods were not tested on this problem set, but the results of Pitha and Jones [10] on similar spectroscopic problems indicated that the performance of DLS was superior to that of the Fletcher-Powell method for such problems. (Hartley's method was not tested by Pitha and Jones.)

In conclusion, for the types of problems dealt with, Hartley's method and MDLS proved to be superior to the other techniques tested. Except for the two problems cited above, Hartley's method and MDLS seemed to be comparable with respect to efficiency in obtaining solutions. MDLS has a theoretical advantage over Hartley's method in that it can be applied to problems in which matrix singularity rules out Hartley's method, but no such problems were actually tested in this study.

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