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# A Homotopy Based Approach to Unconstrained Optimization

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## 1. Introduction

We consider the problem of finding the minimum value of a real valued function $f$ defined on $R^n$ from a homotopic point of view. Davidenko [5] approached this problem by embedding the gradient of $f$, denoted by $F$, into a family of operators and solving a resulting differential equation to obtain a stationary point of $f$ (see Broyden [4] for a discussion of this technique with further references). Boggs [2] examined the use of A-stable integration techniques with this approach and developed specific algorithms for solving the system $F(x) = 0$.

In Section 2 we use the Davidenko embedding method with the homotopy

$$H(t, x) = e^{-t}(x - x^0) + (1 - e^{-t})F(x), \qquad t \geq 0.$$

The corresponding differential equation is then approximated in Section 3, using Euler's rule, to obtain the discrete iteration formula

$$(1.1) \qquad x^{k+1} = x^k - [(1 - \lambda_k)I + \lambda_k F_x(x^k)]^{-1}F(x^k), \qquad \lambda_k \in R.$$

Convergence properties of this iteration scheme for appropriately chosen direction parameters $\lambda_k$ are then developed.

In Section 4 the convergence properties of (1.1) are considered in the case where $f$ is a quadratic function and the Hessian matrix $F_x(x^k)$ is approximated by a matrix that satisfies the secant (quasi-Newton) relation. A quadratic termination property is developed that is similar to that of some variable metric methods. Section 5 examines the choice of direction parameter and develops several global convergence results.

Formula (1.1) is an iteration scheme containing the direction parameter $\lambda_k$ which relates the gradient and Newton directions. A similar formula of the form

$$x^{k+1} = x^k - [\mu_k I + F_x(x^k)]^{-1} F(x^k), \qquad \mu_k \geq 0$$

was developed by Levenberg [11] and by Marquardt [13] for least squares estimation problems. The Levenberg-Marquardt type of algorithm for minimization problems was also considered by Goldfeld, Quandt and Trotter [9] and by Luenberger [12, p. 157]. Hebden [10] further developed the algorithm due to Goldfeld et al. using an approach which is particularly suited for large systems when second derivatives are available. A related "dogleg" strategy was developed by Powell [19, 20, 21] and modified by Dennis and Mei [6]. Another approach based on the gradient path corresponding to the local quadratic approximation of $f$ was developed by Vial and Zang [25].

The dampened version of iteration formula (1.1),

$$x^{k+1} = x^k - \alpha_k [(1 - \lambda_k) I + \lambda_k F_x(x^k)]^{-1} F(x^k),$$

is equivalent for $0 < \lambda_k \leq 1$ to the dampened version of the Levenberg-Marquardt formula,

$$x^{k+1} = x^k - r_k [\mu_k I + F_x(x^k)]^{-1} F(x^k),$$

where $\mu_k = (1 - \lambda_k)/\lambda_k$ and $r_k = \alpha_k/\lambda_k$. However, the analysis of this paper will not impose such a restriction on $\lambda_k$. In fact, nonpositive values of $\lambda_k$ and particularly $\lambda_k = 0$, which gives the gradient direction, might be desirable for (1.1) at a given iteration depending on the eigenvalues of $F_x(x^k)$. This differs from the motivation and implementation of the Levenberg-Marquardt formula, see [9,10,11,13].

## 2. *Derivation*

Let $f : R^n \to R$ and consider the unconstrained optimization problem

$$\text{minimize } f(x) \quad \text{over} \quad x \in R^n.$$

In order to solve this problem we let $F(x)$ be the gradient of $f$ at $x$ and consider the system

(2.1) $$F(x) = 0.$$

An approach to solving (2.1) is to embed the operator $F$ into a family of operators $H(s, \cdot)$ with parameter $s$ and solve a corresponding differential equation. To this end we assume that $F$ has a locally Lipschitz continuous (Fréchet) derivative $F_x$.

Following the development of Meyer [14] we let

(2.2) $$H(s,x) = a(s)G(x) + b(s)F(x), \qquad 0 \leq s \leq 1.$$

Here we assume $a, b : [0, 1] \to R$ and $G : R^n \to R^n$ are twice differentiable and chosen so that $H(1, x) = F(x)$ and $H(0, x^0) = 0$ for some known $x^0 \in R^n$.

If $x(s)$ is a solution of the equation $H(s, x) = 0$ such that $H_x(s, x(s))$ is nonsingular for all $s \in [0, 1]$ then, by the implicit function theorem, $x(s)$ satisfies

$$\dot{x} = H_x(s, x)^{-1} H_s(s, x) \qquad x(0) = x^0. \tag{2.3}$$

Conversely, if $x(s)$ is a solution of (2.3) on $[0, 1]$, then $\frac{dH}{ds}(s, x(s)) = 0$ for $s \in [0, 1]$. Hence

$$H(1, x(1)) = H(0, x^0) = 0$$

and so $x(1)$ is a root of $F(x) = 0$. Thus system (2.1) can be solved by embedding $F$ into the family of operators (2.2) and integrating the corresponding differential equation (2.3).

Conditions for existence and uniqueness of solutions of the differential equation (2.3) on $[0, 1]$ are well-known, in particular see Meyer [14, Section 1].

The particular homotopy we consider is

$$H(s, x) = (1 - s)(x - x^0) + sF(x), \qquad 0 \leq s \leq 1. \tag{2.4}$$

The change of variable $s = 1 - e^{-t}$ gives the homotopy

$$H(t, x) = e^{-t}(x - x^0) + (1 - e^{-t})F(x), \qquad t \geq 0, \tag{2.5}$$

and the homotopies (2.4) and (2.5) are equivalent for $s \in [0, 1)$ and $t \geq 0$.

Letting $t \to +\infty$, the solution $x(t)$ corresponding to (2.5) approaches a root of $F(x) = 0$. Recalling that

$$(2.6) \qquad H(t, x(t)) = 0,$$

and letting $x' = \frac{dx}{dt}$ we calculate

$$(2.7) \qquad \frac{dH}{dt} = H_t + H_x x'$$

$$(2.8) \qquad = [-e^{-t}(x - x^0) + e^{-t}F(x)] + [e^{-t}I + (1 - e^{-t})F_x(x)]x' = 0.$$

By (2.6) and (2.8) we obtain the differential equation

$$(2.9) \qquad x' = -[e^{-t}I + (1 - e^{-t})F_x(x)]^{-1}F(x), \qquad t \geq 0, \quad x(0) = x^0.$$

The motivation for considering the homotopy (2.5) with corresponding differential equation (2.9) on the unbounded interval $t \geq 0$ is to avoid undue accuracy in calculating the approximation to the solution $x(t)$ of the differential equation as $t$ approaches its limit. This accuracy for $x(1)$ is necessary when solving equation (2.3) on $[0, 1]$, (see Boggs [2]).

## 3. The iteration formula and convergence for the general case

The differential equation (2.9) motivates (using Euler's rule) the iteration formula

$$(3.1) \qquad x^{k+1} = x^k - [e^{-t_k}I + (1 - e^{-t_k})F_x(x^k)]^{-1}F(x^k).$$

By writing $\lambda_k = 1 - e^{-t_k}$ equation (3.1) becomes

$$x^{k+1} = x^k - [(1 - \lambda_k)I + \lambda_k F_x(x^k)]^{-1} F(x^k). \tag{3.2}$$

Here $\lambda_k$ is chosen by an appropriate selection rule, an example of which can be described as follows: Let $h : R \to R$ be a twice continuously differentiable function satisfying

$$h(1) = 1, \qquad h'(1) = 0 \tag{3.3}$$

Define then the sequence $\{\lambda_k\}$ by

$$\lambda_{k+1} = h(\lambda_k). \tag{3.4}$$

For example, if we can take

$$h(\lambda) = 1 - \alpha(\lambda - 1)^2, \qquad 0 < \alpha < 1, \tag{3.5}$$

with $|\lambda_0 - 1| \leq 1$, the iterates of (3.4) converge (quadratically) to 1.

In the following we shall deal with rates of convergence of sequences. In this connection we introduce Q- and R-factors for $\{x^k\} \subset R^n$, a sequence converging to $\bar{x}$. For every $p \geq 1$ we define the <u>Q-factors</u> of $\{x^k\}$ as

$$
(3.6)\quad Q_p\{x^k\} = \begin{cases} 0, & \text{if } x^k = \bar{x} \text{ for all but finitely many } k, \\ \overline{\lim\limits_{k\to\infty}} \dfrac{\|x^{k+1} - \bar{x}\|}{\|x^k - \bar{x}\|^p}, & \text{if } x^k \neq \bar{x} \text{ for all but finitely many } k, \\ +\infty, & \text{otherwise} \end{cases}
$$

Similarly, the numbers

$$
(3.7)\qquad R_p\{x^k\} = \begin{cases} \overline{\lim\limits_{k\to\infty}} \|x^k - \bar{x}\|^{1/k}, & \text{if } p = 1, \\ \overline{\lim\limits_{k\to\infty}} \|x^k - \bar{x}\|^{1/(p)^k}, & \text{if } p > 1, \end{cases}
$$

are called the R-factors of $\{x^k\}$.

When $Q_1\{x^k\} = 0$, the sequence $\{x^k\}$ is said to have Q-superlinear rate of convergence. If $0 < Q_2\{x^k\} < +\infty$, then $\{x^k\}$ has Q-quadratic rate of convergence. Similarly, if $R_1\{x^k\} = 0$, the rate of convergence is said to be R-superlinear and if $0 < R_2\{x^k\} < 1$, the rate is R-quadratic. The relationship between Q- and R-factors and the corresponding convergence rates have been examined by Ortega and Rheinboldt [17]. In particular, Q-quadratic (superlinear) convergence implies R-quadratic (superlinear) convergence (see also Tapia [23]).

The local convergence of the iteration (3.2) follows from the "consistent approximation" results of Ortega and Rheinboldt [17, p. 357], as stated below.

*Theorem 3.1. Let* $x^*$ *be a solution of* $F(x) = 0$ *for which* $F_x(x^*)$ *is nonsingular, and let* $N$ *be a sufficiently small neighborhood of* $x^*$. *If* $x^0 \in N$ *and* $\{\lambda_k\}$ *are chosen sufficiently close to 1, then the* *iterates of (3.2) remain in* $N$ *and converge to* $x^*$. *Moreover, if* $\lim_{k \to \infty} \{\lambda_k\} = 1$, *then the iterates of (3.2) converge to* $x^*$ *in a Q-superlinear manner.*

In order to further analyze the rate of convergence of the iteration (3.2) using a parameter selection function (3.4) we introduce the operator $S : R^{n+1} \to R^n$ defined by

$$S(x, \lambda) = x - [(1 - \lambda)I + \lambda F_x(x)]^{-1}F(x) \tag{3.8}$$

and the operator $T : R^{n+1} \to R^{n+1}$ defined by

$$T(x, \lambda) = (S(x, \lambda), h(\lambda)). \tag{3.9}$$

Then the formulas (3.2) and (3.4) are equivalent to

$$(x^{k+1}, \lambda_{k+1}) = T(x^k, \lambda_k), \tag{3.10}$$

where $(x^0, \lambda_0)$ are given. Next we have

*Proposition 3.2. The operator* $S$ *has a fixed point at* $x^*$ *for some fixed* $\lambda$ *if and only if* $F(x^*) = 0$.

*Proof.* If $F(x^*) = 0$, then from (3.8) we have $S(x^*, \lambda) = x^*$ for all $\lambda$. If $S(x^*, \lambda) = x^*$ in (3.8) the nonsingularity of $[(1 - \lambda)I + \lambda F_x(x^*)]^{-1}$ gives $F(x^*) = 0$. □

From here on we assume that $x^*$ is a solution of system (2.1) and take $\lambda_0$ and $h$ in (3.4) to be chosen so that the sequence $\{\lambda_k\}$ converges to 1 and such that the matrix $[(1 - \lambda_k)I + \lambda_k F_x(x)]$ is invertible for $x$ in an appropriate neighborhood of $x^*$. Let $S_1$ and $S_2$ denote the derivative of the operator $S$ with respect to $x$ and $\lambda$, respectively.

Proposition 3.3. If the matrix $[(1 - \lambda)I + \lambda F_x(x^*)]$ is invertible for some value $\lambda$, then $S_2(x^*, \lambda) = 0$.

Proof. From (3.8) we have

$$[(1 - \lambda)I + \lambda F_x(x)](x - S(x, \lambda)) = F(x).$$

Thus by differentiating with respect to $\lambda$ we obtain

$$[- I + F_x(x)](x - S(x, \lambda)) - [(1 - \lambda)I + \lambda F_x(x)]S_2(x, \lambda) = 0,$$

and

$$S_2(x, \lambda) = [(1 - \lambda)I + \lambda F_x(x)]^{-1}[- I + F_x(x)](x - S(x, \lambda)).$$

By Proposition 3.2, $F(x^*) = 0$ implies $(x^* - S(x^*, \lambda)) = 0$ which completes the proof. □

Proposition 3.4. Let $\{\lambda_k\}$ converge to 1. Then

$$\lim_{k \to \infty} \{S_1(x^*, \lambda_k)\} = 0.$$

<u>Proof</u>.

$$S_1(x^*, \lambda)(\eta) = \lim_{\tau \to 0} \frac{S(x^* + \tau\eta, \lambda) - S(x^*, \lambda)}{\tau}$$

$$= \lim_{\tau \to 0} \left\{ \eta - \frac{[(1-\lambda)I+\lambda F_x(x^*+\tau\eta)]^{-1}F(x^*+\tau\eta) - [(1-\lambda)I+\lambda F_x(x^*)]^{-1}F(x^*)}{\tau} \right\}$$

$$= \lim_{\tau \to 0} \left\{ \eta - [(1-\lambda)I+\lambda F_x(x^*+\tau\eta)]^{-1} \frac{F(x^*+\tau\eta)-F(x^*)}{\tau} \right\},$$

since $F(x^*) = 0$. Hence

$$S_1(x^*, \lambda_k)(\eta) = \eta - [(1 - \lambda_k)I + \lambda_k F_x(x^*)]^{-1}F_x(x^*)\eta.$$

Taking $\{\lambda_k\}$ converging to 1 completes the proof. □

We are now able to obtain our result on the convergence rate of the iteration defined by (3.2) and (3.4).

<u>Theorem 3.5. Let</u> $h$ <u>satisfy condition (3.3) and choose</u> $\lambda_0$ <u>so that the sequence defined by (3.4) converges to 1. Then the sequence</u> $\{(x^k, \lambda_k)\}$ <u>defined by (3.2) and (3.4) converges locally to</u> $(x^*, 1)$ <u>and this convergence is Q-quadratic</u>.

<u>Proof</u>. Let $DT$ and $D^2T$ denote the first and second derivatives of the operator $T$, defined by (3.9). By (3.3) we have

$$h'(1) = 0$$

and hence Proposition 3.3 and 3.4 together with the continuity of $S_1$ imply $DT(x^*, 1) = 0$. Therefore, Taylor's Theorem and the Schwarz inequality gives

$$\|(x^{k+1},\lambda_{k+1})-(x^*,1)\| = \|T(x^k,\lambda_k)-T(x^*,1)\|$$

$$\leq \frac{1}{2} \|D^2T(x^*+\theta(x^*-x^k),1+\psi(1-\lambda_k))\|\|(x^k,\lambda_k)-(x^*,1)\|^2$$

for some $\theta$ and $\psi$ between 0 and 1. Hence we have

$$(3.11) \qquad \overline{\lim_{k\to\infty}} \frac{\|(x^{k+1}, \lambda_{k+1}) - (x^*, 1)\|}{\|(x^k, \lambda_k) - (x^*, 1)\|^2} < +\infty$$

and from (3.11) and (3.6) it follows that the rate of convergence is Q-quadratic. □

As was pointed out by Tapia [23], the above result does not imply that the sequence $\{x^k\}$ itself converges Q-quadratically. However, following Tapia, we note that

$$\|x^k - x^*\| \leq \|(x^k, \lambda_k) - (x^*, 1)\|$$

and so definition (3.7) and Theorem 3.5 give the following result.

Corollary 3.6. Suppose $h$ and $\lambda_0$ are as in Theorem 3.5 and let the sequence $\{(x^k, \lambda_k)\}$ be defined by (3.2) and (3.4). Then the sequence $\{x^k\}$ converges locally to $x^*$ and the rate of convergence is R-quadratic.

We may remark here that, by Theorems 3.1 and 3.5, the iteration formula (3.2) derived from the homotopy (2.5) has a rate of convergence comparable to Newton's method, which is Q-quadratic, in a neighborhood of a root of (2.1).

## 4. Convergence for quadratic functions

As is well known, the evaluation of the Hessian matrix $F_x(x^k)$ in formula (3.2) can be an expensive calculation. We therefore consider the convergence question where the Hessian matrix is approximated in a quasi-Newton manner, see for example [3, 16]. In this approach we approximate $F_x(x^k)$ by a square matrix $A_k$ and define our iteration formula by

$$(4.1) \qquad x^{k+1} = x^k - [(1 - \lambda_k)I + \lambda_k A_k]^{-1} F(x^k).$$

We assume that there is an interval $J$, possibly unbounded, such that the matrix $[(1 - \lambda)I + \lambda A_k]^{-1}$ is positive definite for all $\lambda \in J$ and that the function $f(x^{k+1})$ as a function of $\lambda$ achieves its minimum over all $\lambda$ in $J$ at some point $\lambda_k$ interior to $J$. (If $A_k$ is symmetric the interval $J$ can be completely described in terms of the eigenvalues of $A_k$.) Then at $\lambda = \lambda_k$ we have

$$\frac{d}{d\lambda} f(x^{k+1}) = 0,$$

or

$$(4.2) \qquad (1 - \lambda_k) F(x^{k+1})^T (I - A_k)[(1 - \lambda_k)I + \lambda_k A_k]^{-2} F(x^k) = 0.$$

Let $\gamma^{k+1} = F(x^{k+1}) - F(x^k)$ and $p^{k+1} = x^{k+1} - x^k$. It is known [7,16] that the quasi-Newton iteration formula

$$x^{k+1} = x^k - B_k F(x^k)$$

will converge to a stationary point of the quadratic function $f : R^n \to R$

in $n + 1$ iterations if the matrix $B_k$ is updated at each iteration so that it satisfies the secant relation

$$(4.3) \qquad B_k \gamma^i = p^i, \qquad i = 1, 2, \ldots, k.$$

If $f$ is quadratic with Hessian matrix $Q$, then equation (4.3) is automatically satisfied for $B_k = Q^{-1}$. The secant relation also holds if $B_k$ is updated by the symmetric rank one formula, see [16]. We now derive a similar quadratic termination result for the iteration (4.1). This result was motivated by the work of Vial and Zang [25].

Theorem 4.1. *Suppose $f$ is quadratic and $x^{k+1}$ is given by formula (4.1) where $\lambda_k \in J$ satisfies (4.2). If $B_k = A_k^{-1}$ exists and satisfies the secant relation (4.3), then either $p^{k+1}$ is linearly independent of $p^1, \ldots, p^k$ or else $F(x^{k+1}) = 0$.*

*Proof.* Suppose $p^{k+1}$ is linearly dependent on $p^1, \ldots, p^k$. Then there exist numbers $\beta_1, \ldots, \beta_k$, not all zero, such that

$$(4.4) \qquad p^{k+1} = \sum_{i=1}^{k} \beta_i p^i.$$

If $f$ is the quadratic function $f(x) = a + b^T x + \frac{1}{2} x^T Q x$, we have $\gamma^i = Qp^i$ and hence

$$(4.5) \qquad \gamma^{k+1} = Qp^{k+1} = \sum_{i=1}^{k} \beta_i Q p^i = \sum_{i=1}^{k} \beta_i \gamma^i.$$

Since $A_k^{-1}$ satisfies the secant relation (4.3), equations (4.4) and (4.5) imply

$$p^{k+1} = \sum_{i=1}^{k} \beta_i A_k^{-1}\gamma^i = A_k^{-1} \sum_{i=1}^{k} \beta_i \gamma^i = A_k^{-1}\gamma^{k+1}.$$

Hence we obtain

$$p^{k+1} = A_k^{-1}[F(x^{k+1}) - F(x^k)]. \tag{4.6}$$

However, from equation (4.1) we have

$$p^{k+1} = - [(1 - \lambda_k)I + \lambda_k A_k]^{-1} F(x^k). \tag{4.7}$$

Equations (4.6) and (4.7) then give

$$\begin{aligned} F(x^{k+1}) &= F(x^k) - A_k[(1 - \lambda_k)I + \lambda_k A_k]^{-1} F(x^k) \\ &= (I - A_k[(1 - \lambda_k)I + \lambda_k A_k]^{-1})F(x^k) \\ &= (1 - \lambda_k)(I - A_k)[(1 - \lambda_k)I + \lambda_k A_k]^{-1} F(x^k) \\ &= (1 - \lambda_k)[(1 - \lambda_k)I + \lambda_k A_k](I - A_k)[(1 - \lambda_k)I + \lambda_k A_k]^{-2} F(x^k), \end{aligned}$$

since both $I$ and $A_k$ commute with $[(1 - \lambda_k)I + \lambda_k A_k]$. Hence it follows that

$$\begin{aligned} &F(x^{k+1})^T[(1 - \lambda_k)I + \lambda_k A_k]^{-1} F(x^{k+1}) = \\ &(1 - \lambda_k)F(x^{k+1})^T(I - A_k)[(1 - \lambda_k)I + \lambda_k A_k]^{-2} F(x^k) = 0, \end{aligned} \tag{4.8}$$

since $\lambda_k$ satisfies (4.2). But $\lambda_k \in J$ implies that the matrix $[(1-\lambda_k)I + \lambda_k A_k]^{-1}$ is positive definite and therefore (4.8) yields $F(x^{k+1}) = 0$, as asserted. □

Since there can be at most $n$ linearly independent vectors in $R^n$ the following result is valid.

Corollary 4.2. *Suppose that for each* $k = 1, 2, \ldots, n$, $A_k^{-1}$ *satisfies the secant relation (4.3) and it is possible to choose* $\lambda_k$ *satisfying equation (4.2) and such that the matrix* $[(1-\lambda_k)I + \lambda_k A_k]^{-1}$ *is positive definite. Then the iteration formula (4.1) will obtain a stationary point of a quadratic function in at most* $n+1$ *iterations and* $A_n = Q$.

Remark. The results of sections 3 and 4 are also valid for the corresponding Levenberg-Marquardt algorithms. In this case equation (4.2) becomes

$$F(x^{k+1})^T[\mu_k I + A_k]^{-2}F(x^k) = 0.$$

The proofs of these results follow directly along the lines of those above.

## 5. Discussion of the direction parameter and some global convergence results.

There are a variety of possible ways for choosing the direction parameter $\lambda_k$ in iteration formulas (3.2) or (4.1). One approach is to choose $\lambda_k$ by a *predetermined* rule which is based on previous information about the system. This type of selection is fundamental in many of the Levenberg-Marquardt or "dogleg" strategies that have been developed, see [6,10,11,19].

One could also use formula (4.2) restricting $\lambda_k$ to the interval J where the matrix $[(1 - \lambda)I + \lambda A_k]^{-1}$ is positive definite. The following results characterize this interval for symmetric matrices $A_k$.

Proposition 5.1. Suppose A is symmetric. Then the following are equivalent:

(i) The matrix $[(1 - \lambda)I + \lambda A]$ is invertible for all $0 \leq \lambda \leq 1$,

(ii) The matrix $[(1 - \lambda)I + \lambda A]$ is positive definite for all $0 \leq \lambda \leq 1$,

(iii) A is positive definite.

Proof. Write $A = U\Sigma U^T$ where $UU^T = I$ and $\Sigma$ is a diagonal matrix with diagonal elements $\sigma_1, \sigma_2, \ldots, \sigma_n$, the eigenvalues of A, see [13, p. 36]. Then the matrix

$$(5.1) \qquad [(1 - \lambda)I + \lambda A] = U[(1 - \lambda)I + \lambda\Sigma]U^T$$

has eigenvalues $1 - \lambda + \lambda\sigma_i$ for $i = 1,2,\ldots,n$. Considering the determinant in (5.1) we see that $[(1 - \lambda)I + \lambda A]$ is invertible iff $1 - \lambda + \lambda\sigma_i \neq 0$ for all $i = 1,2,\ldots,n$, i.e. iff $\lambda \neq 1/(1 - \sigma_i)$ for all $i = 1,2,\ldots,n$. But $1/(1 - \sigma_i) \notin [0,1]$ iff $\sigma_i > 0$. Consequently, A is positive definite iff $\sigma_i > 0$ for $i = 1,2,\ldots,n$. Hence (i) and (iii) are equivalent. To see that (ii) and (iii) are equivalent note that $1 - \lambda + \lambda\sigma_i > 0$, i.e. $1 > \lambda(1 - \sigma_i)$, for all $\lambda \in [0,1]$ iff $\sigma_i > 0$. □

Clearly the interval $J$ contains $\lambda = 1$ iff $A$ is positive definite. Note also that $\lambda = 0$ *is in* $J$ *for every* $A$. Therefore the gradient direction is a feasible direction at each iteration; this is *not the case* in the Levenberg-Marquardt algorithms.

<u>Proposition 5.2. Suppose</u> $A$ <u>is symmetric and its eigenvalues are</u> $\sigma_1 \le \sigma_2 \le \dots \le \sigma_n$. <u>Let</u> $J$ <u>be the set of real numbers</u> $\lambda$ <u>such that the matrix</u> $[(1-\lambda)I + \lambda A]^{-1}$ <u>is positive definite.</u>

<u>(i) If</u> $\sigma_1 = \sigma_n = 1$, <u>then</u> $J = (-\infty, +\infty)$.

<u>(ii) If</u> $\sigma_1 < \sigma_n \le 1$, <u>then</u> $J = (-\infty, \frac{1}{1-\sigma_1})$.

<u>(iii) If</u> $\sigma_1 < 1 < \sigma_n$, <u>then</u> $J = (\frac{1}{1-\sigma_n}, \frac{1}{1-\sigma_1})$.

<u>(iv) If</u> $1 \le \sigma_1 < \sigma_n$, <u>then</u> $J = (\frac{1}{1-\sigma_n}, +\infty)$.

<u>Proof</u>. Take $A = U\Sigma U^T$ as the proof of Proposition 5.1. Note that if $\sigma_i = 1$ then $1 - \lambda + \lambda\sigma_i = 1$ for all $\lambda$. Hence part (i) is valid.

To prove part (ii) let $\sigma_1 \le \sigma_i < 1$, then $1 - \sigma_1 \ge 1 - \sigma_i > 0$. So, $1/(1-\sigma_i) \ge 1/(1-\sigma_1) > 0$. Therefore, if $\lambda < 1/(1-\sigma_1) \le 1/(1-\sigma_i)$, we have $\lambda(1-\sigma_i) < 1$ or $0 < 1 - \lambda + \lambda\sigma_i$. For the converse note that if $\lambda \ge 1/(1-\sigma_1)$ we have $0 \ge 1 - \lambda + \lambda\sigma_1$ which implies that $[(1-\lambda)I + \lambda A]$ has a negative eigenvalue.

To prove part (iv) we consider $1 < \sigma_i \le \sigma_n$. Then $0 \ge 1 - \sigma_i \ge 1 - \sigma_n$ and so $1/(1-\sigma_i) \le 1/(1-\sigma_n) < 0$. Therefore, if $\lambda > 1/(1-\sigma_n) \ge 1/(1-\sigma_i)$ we have $\lambda(1-\sigma_i) < 1$ or $0 < 1 - \lambda + \lambda\sigma_i$. For the converse note that if $\lambda \le 1/(1-\sigma_n)$ we have $\lambda(1-\sigma_n) \ge 1$ or $0 \ge 1 - \lambda + \lambda\sigma_n$ which implies $[(1-\lambda)I + \lambda A]$ has a negative eignevalue.

The proof of part (iii) follows immediately from the above two cases. ☐

From the proof of Proposition 5.2 one can see that the magnitude of the vector

$$x^{k+1}(\lambda) = x^k - [(1 - \lambda)I + \lambda A_k]^{-1}F(x^k)$$

can be expected to increase, usually without bound, as $\lambda$ approaches either end point of $J$. In this case the continuity of $F$ with respect to $\lambda$ would indicate the existence of a minimum of this function in $J$ - that is, a value of $\lambda$ which satisfies (4.2).

Another approach which would avoid solving equation (4.2) is to use a search technique to find a number that approximates the value of $\lambda_k$ for which $f[x^{k+1}(\lambda)]$ achieves its minimum over $J$. This approach for determining $\lambda_k$ appears to have promise computationally since it produces an approximation to the best direction available when using a positive definite matrix in the iteration formula.

This is further supported by the following global convergence property for the dampened iteration formula

$$(5.3) \qquad x^{k+1} = x^k - \alpha_k[(1 - \lambda_k)I + \lambda_k F_x(x^k)]^{-1}F(x^k) \ .$$

The dampening term $\alpha_k$ is introduced since the undampened version, as in Newton's method, need not involve a descent direction for a general $f$ except in an appropriate neighborhood of $x^*$. For the next results we let $J(x)$ be the set of real numbers $\lambda$ for which the matrix $[(1 - \lambda)I + \lambda F_x(x)]^{-1}$ is positive definite. Since $F_x(x)$ is symmetric and the eigenvalues of a matrix vary continuously with the components, Proposition 5.2 shows that $J(x)$ is an interval which depends continuously on $x$. Hence there exists a continuous selection function $\lambda: R^n \to R$ such that $\lambda(x) \in J(x)$ for all $x$ [15, Th. 2.1]. Indeed, there are many such functions and we will demonstrate one shortly. Using such a function $\lambda(x)$, iteration formula (5.3) can be employed as follows:

i) Given a point $x^k$ set $\lambda_k = \lambda(x^k)$ ;

ii) Define:

$$x^{k+1}(\lambda_k,\alpha) = x^k - \alpha[(1-\lambda_k)I + \lambda_k F_x(x^k)]^{-1}F(x^k)$$

and let $\alpha_k$ minimize $f[x^{k+1}(\lambda_k,\alpha)]$ over $\alpha \geq 0$ ;

iii) Set $x^{k+1} = x^{k+1}(\lambda_k,\alpha_k)$ .

Theorem 5.3. Suppose $\lambda(x)$ is a continuous selection function for $J$ and let the sequence $\{x^k\}$ be defined by iteration formula (5.3) where we set $\lambda_k = \lambda(x^k)$ and let $\alpha_k$ minimize $f[x^{k+1}(\lambda_k,\alpha)]$ over $\alpha \geq 0$. Then the limit of any convergent subsequence of $\{x^k\}$ is a solution of (2.1). In particular, if $\{x^k\}$ is bounded, it will have limit points and each of these will be a solution of (2.1).

Proof. Let $D: R^n \to R^{2n}$ be a map which associates to every point $x^k$ the pair $(x^k,d^k)$ where $d^k$ is the direction

$$d^k = -[(1-\lambda_k)I + \lambda_k F_x(x^k)]^{-1}F(x^k) .$$

Note that since $\lambda_k \in J(x^k)$, $d^k$ is a direction of descent for $f$. Further, since $\lambda(x)$ is continuous, the map D is a continuous point-to-set map. Let $S: R^{2n} \to R^n$ be a point-to-set map defined by

$$S(x,d) = \{y : y = x + \alpha d \text{ for some } \alpha \geq 0,\ f(y) = \min_{0 \leq \alpha < \infty} f(x+\alpha d)\}.$$

Then $\lambda_k \in J(x^k)$ implies $d^k \neq 0$ and so $S$ is a closed map on the range of $D$ [12, p.146]. Hence the composite map SoD is closed and the limit of any convergent subsequence of the iteration

$$x^{k+1} = \mathrm{SoD}(x^k)$$

is a solution of (2.1) [12, p.125]. Weierstrass' Theorem that $R^n$ is sequentially compact shows that if $\{x^k\}$ is bounded it has a convergent subsequence. This completes the proof. □

The success which quadratic approximation of functions has enjoyed in optimization techniques motivates the following example of a continuous selection function $\lambda(x)$ . Approximate the function $f[x^{k+1}(\lambda)]$ by a quadratic function whose coefficients are determined by three values of $\lambda$ which depend continuously on the endpoints of the interval $J(x^k)$ , such as the values $\lambda_1 = 0$, $\lambda_2 = (0.1)\gamma$, where $\gamma = \max\{-\varepsilon, \frac{1}{1-\sigma_n}\}$ , and $\lambda_3 = (0.1)\delta$, where $\delta = \min\{\xi, \frac{1}{1-\sigma_1}\}$ for specified $\varepsilon$, $\xi$ . Then let $\lambda(x^k)$ be the minimum point for this quadratic function or an appropriate bound in case the minimum point does not lie in $J(x^k)$ or lies too close to one end point of $J(x^k)$ . Other approaches for defining the selection function $\lambda(x)$ are motivated by the techniques described in [6,10,19,21].

We now consider iteration formula (5.3) where the dampening term $\alpha_k$ is not an exact minimization step size. Instead we use an Armijo step size procedure which is based on sufficient function value decrease [1]. For this result we let $\|\cdot\|$ denote the Euclidean norm of $R^n$ .

*Theorem 5.4. Suppose* $\lambda(x)$ *is a continuous selection function for J and define*

$$S(x,\delta) = \{x^\alpha : x^\alpha = x - \alpha[(1-\lambda(x))I+\lambda(x)F_x(x)]^{-1}F(x),$$
$$\alpha > 0,\ f(x^\alpha) - f(x) \leq -\delta||F(x)||^2\}.$$

*Assume the following conditions hold:*

i) *The initial point* $x^0$ *is given and is such that the set*

$$S(x^0) = \{x: f(x) \leq f(x^0)\}$$

*is bounded.*

ii) *There exists a constant K such that*

$$||F(y)-F(x)|| \leq K||y-x||$$

*for all* $x,y \in S(x^0)$.

*Then there exists a* $\delta > 0$ *such that for any* $x \in S(x^0)$ *the set* $S(x,\delta)$ *is a nonempty subset of* $S(x^0)$. *Further, for any such* $\delta$ *and any sequence* $\{x^k\}$ *such that*

$$x^{k+1} \in S(x^k,\delta), \qquad k = 0,1,2,\ldots,$$

*the sequence has at least one convergent subsequence and the limit of any convergent subsequence is a solution of (2.1).*

Proof. We let $P(x)$ denote the matrix

$$P(x) = [(1-\lambda(x))I + \lambda(x)F_x(x)]^{-1},$$

and $||P(x)||$ is the operator norm induced by the Euclidean norm on $R^n$. Thus $||P(x)||$ is a continuous real valued function on $R^n$ and hence is bounded on the closure of $S(x^0)$, say

$$||P(x)|| \leq M$$

for all $x \in S(x^0)$. Similarly, there is an $N > 0$ such that

$$||P(x)^{-1}|| \leq N$$

for all $x \in S(x^0)$. Take $\bar{\delta} = (4KM^2N^2)^{-1}$ and let $x \in S(x^0)$. For any fixed $\alpha$ the mean value theorem implies there is a point $\bar{x}$ satisfying

$$||\bar{x} - x|| \leq ||x^\alpha - x||$$

and such that

$$\begin{aligned} f(x^\alpha) - f(x) &= (x^\alpha - x)^T F(\bar{x}) \\ &= -\alpha[P(x)F(x)]^T[F(x) + F(\bar{x}) - F(x)] \\ &= -\alpha F(x)^T P(x)F(x) - \alpha F(x)^T P(x)[F(\bar{x}) - F(x)] \\ &\leq -\alpha F(x)^T P(x)F(x) + \alpha||F(x)||MK||x^\alpha - x|| \\ &\leq -\alpha F(x)^T P(x)F(x) + \alpha^2 KM^2||F(x)||^2, \end{aligned}$$

using (ii). Since $P(x)$ is a symmetric positive definite matrix for each $x$ we can write $P(x) = G^T G$ for some matrix $G$. Letting $\rho(A)$ denote the spectral radius of the matrix $A$ we have the following inequality holding for each $y \in R^n$ [24,p.11]:

$$|y^T P(x) y| = ||Gy||^2 \geq \frac{||y||^2}{||G^{-1}||^2}$$

$$= \frac{||y||^2}{\rho(G^{-1}G^{-1T})} = \frac{||y||^2}{\rho(P^{-1}(x))}$$

$$= \frac{||y||^2}{||P^{-1}(x)||} \geq \frac{||y||^2}{N}.$$

Hence we have

$$f(x^\alpha) - f(x) \leq -\frac{\alpha}{N}||F(x)||^2 + \alpha^2 KM^2 ||F(x)||^2$$

$$= -\bar{\delta}||F(x)||^2$$

for $\alpha = (2KM^2N)^{-1}$. Thus $S(x,\bar{\delta})$ is not empty.

Now, let $\delta > 0$ be such that $S(x,\delta)$ is nonempty for any $x \in S(x^0)$ and suppose the sequence $\{x^k\}$ is such that

$$x^{k+1} \in S(x^k,\delta), \qquad k = 0,1,2,\ldots.$$

Then the definition of $S(x,\delta)$ implies the sequence $\{f(x^k)\}$, which is bounded below by its minimum vlaue, is monotone nonincreasing and hence converges. Since

(5.4) $$f(x^{k+1}) - f(x^k) \leq -\delta||F(x^k)||^2 \leq 0,$$

the sequence $\{F(x^k)\}$ converges to the zero vector. The result now follows,since $S(x^0)$ is bounded. □

This result indicates that a good procedure for determining the dampening term is to let $\alpha_k$ be the first number in the sequence $(0.1)^j$, $j = 0,1,2,\ldots$, that satisfies the condition

$$f(x^{k+1}) - f(x^k) \leq \varepsilon\alpha \, ||F(x^k)||^2,$$

for an appropriate small number $\varepsilon > 0$, say $\varepsilon = 0.0001$ as is suggested by Powell [22, (3.5)]. This type of procedure was proposed by Fletcher [8] and is a successful method in practice (see also [17, p.503]). The value $\alpha_k = 1$ is used first since we eventually expect R-quadratic convergence by Corollary 3.6, provided the selection function $\lambda(x)$ approaches the value 1 near the solution. In fact, this would be expected when using either equation (4.2) or the quadratic approximation approach described above since they are designed to obtain the best direction when using unit step length. Thus these selection functions would favor Newton's direction near a solution.

It should be noted, however, that R-linear convergence can be guaranteed for any continuous selection function provided equation (2.1) has a finite number of solutions and the Hessian matrix $F_x(x^*)$ is nonsingular at these points. In fact, under these assumptions the results of Ostrowski ([18], see also [17, Theorems 14.1.5 and 14.1.6]) imply that the sequence $\{x^k\}$ itself will converge to a solution of (2.1) with at least an R-linear rate of convergence. This result follows immediately from those of Ostrowski using equation (5.4).

Theorems 3.5, 5.3 and 5.4 motivate a number of other iteration schemes which should have good convergence properties even when $\lambda_k$, $\alpha_k$ and $F_x(x^k)$ are approximated appropriately. Naturally the success of such schemes depend on how the various details are implemented. However, these results will rely on computational experience and so will be reported separately.

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The problem of finding a local minimum of a real differentiable function is considered from a homotopic point of view. Using the Davidenko embedding method with a particular homotopy, an ordinary differential equation is derived. Solution of this equation by Euler's rule gives rise to an iteration formula for the optimization problem. Convergence and termination properties of this formula are discussed.

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