A NEW ALGORITHM FOR NONLINEAR LEAST SQUARES CURVE FITTING

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1. Introduction and Description of the Method.

In this paper we present a new algorithm for the problem of fitting a given set of tabular data points with a curve in the nonlinear least squares sense. We give convergence theorems for the method and report the results of computational investigations in which the algorithm was tested against currently used minimization techniques.

Let (p_i, y_i), $i = 1,\ldots,M$ be given data, let $x \in E^N$, and suppose we wish to fit a function of the form $g(x;p)$ to the data in such a way that

$$\phi(x) = ||g(x,p) - y||_2^2 = \sum_{i=1}^{M} (g(x;p_i) - y_i)^2$$

is a minimum; i.e. we seek a point $x^* \in E^N$ which minimizes the scalar function ϕ. Now every such relative minimum will be found among the zeros of $\phi'(x)$, the gradient of the ϕ. If we set

$$F(x) \equiv g(x;p) - y ,$$

and

$$G(x) \equiv J_F^T(x)F(x) ,$$

where $J_F(x)$ denotes the $M \times N$ Jacobian matrix of $F = (f_1,\ldots,f_M)^T$, then our task is to find the zeros of $G(x)$ and hence of the gradient $\phi'(x)$.

Let $H_i(x)$ denote the Hessian matrix of f_i at x . By direct calculation we have that

(1) $$J_G(x) = \sum_{k=1}^{M} f_k(x)H_k(x) + J_F(x)^T J_F(x) ,$$

so that Newton's method applied to

(2) $$G(x) = 0$$

is given by

(3) $$x_{n+1} = x_n - [\sum_{k=1}^{M} f_k(x_n)H_k(x_n) + J_F(x_n)^T J_F(x_n)]^{-1} J_F^T(x_n)F(x_n) .$$

The latter formula requires (assuming continuous second partial derivatives of ϕ) the calculation of $M \cdot N \cdot (N+1)/2$ second partial derivatives per iterative step. The Gauss-Newton [12] and Levenberg-Marquardt [12] algorithms are two frequently used attempts to circumvent this difficulty. The former simply drops the term $\sum_{k=1}^{M} f_k(x_n)H_k(x_n)$ and the latter approximates it with a diagonal matrix $\mu_n I$. Both methods work well locally when $||F(x)||$ is very small at a zero of G. For example in [3], we have shown that the Levenberg-Marquardt iteration converges quadratically to x^*, a zero of F, if $\mu_n = O(||F(x_n)||)$ and $J_F(x^*)$ has full rank. Obviously the Gauss-Newton method behaves likewise. When the stationary points have large residuals the Levenberg-Marquardt algorithm can degenerate into an awkward descent method, for then the H_k in (3) are no longer damped out.

In order to approximate the H_k without requiring additional derivative or function evaluations, we propose the following algorithm.

Algorithm 1.1. Let x_n, $J_F(x_n)$ and $F(x_n)$ be given along with M matrices $B_{1,n}, \ldots, B_{M,n}$ each of size $N \times N$. (Initially the $B_{i,o}$ may be chosen to approximate the $H_i(x_o)$ by, say, using first differences or the entries of $J_F(x_n)$.) Obtain

$$(4) \quad x_{n+1} = x_n - [\sum_{k=1}^{M} f_k(x_n) B_{k,n} + J_F(x_n)^T J_F(x_n)]^{-1} J_F(x_n)^T F(x_n)$$

$$= x_n - A_n^{-1} J_F(x_n)^T F(x_n)$$

and compute $J_F(x_{n+1})$ and $F(x_{n+1})$.

Now update the B_i by means of

$$(5)\quad B_{i,n+1} = B_{i,n} + [\nabla f_i(x_{n+1})^T - \nabla f_i(x_n)^T - B_{i,n}(x_{n+1}-x_n)] \frac{(x_{n+1}-x_n)^T}{||x_{n+1}-x_n||_2^2} ,$$

for each $i = 1,\ldots,M$. Continue the process until termination criteria are met.

Remark 1.1. $\nabla f_i(x)$ is just the ith row of $J_F(x)$.

Remark 1.2. Equation (5) is the appropriate generalization [6] of Broyden's "single-rank" approximation to $H_i(x^n)$ [4].

Remark 1.3. The algorithm requires no more function or derivative evaluations than do the Gauss-Newton or Levenberg-Marquardt algorithms; however, more storage space is needed. The additional storage requirement is offset on the one hand by superior local behavior (stability near a root) and on the other hand by a gain in speed of convergence.

2. Convergence Results.

The purpose of this section is to present theorems which characterize the local convergence properties of the algorithm.

The following lemma bounds the error in the Hessian approximations given by (5).

Lemma 1. Let Ω be an open convex neighborhood of x^*, and let $K \geq 0$ be a constant and P be a Frechet differentiable function mapping Ω into E^N such that for every $x \in \Omega$,

$$\text{(L1)} \qquad ||J_P(x^*) - J_P(x)|| \leq K||x^* - x|| .$$

Let B be a real $N \times N$ matrix and let $x, x' \in \Omega$. Define B' by

$$\text{(5')} \qquad B' \equiv B + [P(x') - P(x) - B(x' - x)] \frac{(x'-x)^T}{||x'-x||^2} .$$

Under these hypotheses

$$||B' - J_P(x')|| \leq ||B - J_P(x)|| + 2K(||x - x^*|| + ||x' - x^*||) .$$

If, in addition,

$$\text{(L2)} \qquad ||J_P(x) - J_P(y)|| \leq K||x - y|| ,$$

then

$$||B' - J_P(x')|| \leq ||B - J_P(x)|| + \tfrac{3}{2} K||x' - x|| .$$

<u>Proof</u>.

$$B' - J_p(x') = B - J_p(x) + [P(x') - P(x) - B(x' - x)] \frac{(x'-x)^T}{||x'-x||^2}$$
$$+ J_p(x) - J_p(x')$$
$$= B - J_p(x) + [P(x') - P(x) - J_p(x)(x' - x)] \frac{(x'-x)^T}{||x'-x||^2}$$
$$+ [J_p(x) - B] \frac{(x'-x)(x'-x)^T}{||x'-x||^2} + J_p(x) - J_p(x') .$$

$$||B' - J_p(x')|| \leq ||B - J_p(x)|| \cdot ||I - \frac{(x'-x)(x'-x)^T}{||x'-x||^2}||$$
$$+ ||P(x') - P(x) - J_p(x)(x' - x)||$$
$$\cdot ||x' - x||^{-1} + ||J_p(x) - J_p(x')|| .$$

Now from [4], $||I - \frac{(x'-x)(x'-x)^T}{||x'-x||^2}|| = 1$. If J_p is Lipschitz (L2 holds), the corresponding result is clear. If we only assume the one sided Lipschitz condition L1, then the above reduces to

$$||B' - J_p(x')|| \leq ||B - J_p(x)|| + \sup_{\xi \in (x',x)} ||J_p(x) - J_p(\xi)||$$
$$+ ||J_p(x) - J_p(x')||$$
$$\leq ||B - J_p(x)|| + 2K(||x - x^*|| + ||x' - x^*||)$$

by adding and subtracting $J_p(x^*)$ twice.

<u>Lemma 2</u>. If, for each $i = 1,\ldots,M$, H_i satisfies L1 with constants K_i on a compact convex subset C of Ω then there is a constant γ_1 such that J_G satisfies L_1 with $K = \gamma_1$ on C.

<u>Proof</u>. Let $K = \max K_i$ and select $B \geq ||H_i(x)||$, $B' \geq ||J_F(x)|| = ||J_F(x)^T||$ (see [18]), $B'' \geq ||F(x)||_1$ for every $x \in C$, $i = 1,\ldots,M$. These constants can be chosen because of the continuity of every H_i and the compactness of C. Notice that $M^{\frac{1}{2}}B$, B' serve as Lipschitz constants for J_F and F on C.

Assume that every H_i satisfies L1, then

$$\begin{aligned}
||J_G(x) - J_G(x^*)|| &= ||\Sigma f_i(x)H_i(x) + J_F^T(x)J_F(x) \\
&\qquad - \Sigma f_i(x^*)H_i(x^*) - J_F^T(x^*)J_F(x^*)|| \\
&\leq ||\Sigma[f_i(x) - f_i(x^*)]H_i(x)|| + ||\Sigma f_i(x^*)[H_i(x) - H_i(x^*)]|| \\
&\qquad + ||J_F(x)^T[J_F(x)-J_F(x^*)]||+||[J_F(x)^T-J_F(x^*)^T]J_F(x^*)|| \\
&\leq ||F(x) - F(x^*)|| \cdot (\sum_{i=1}^{M} ||H_i(x)||^2)^{\frac{1}{2}} \\
&\qquad + ||F(x^*)||_1 \max_i ||H_i(x) - H_i(x^*)|| \\
&\qquad + ||J_F(x)^T|| \cdot ||J_F(x) - J_F(x^*)|| \\
&\qquad + ||J_F(x^*)|| \cdot ||J_F(x)^T - J_F(x^*)^T||
\end{aligned}$$

$$\leq (M^{\frac{1}{2}}BB' + B''K + 2B')||x - x^*||$$
$$\equiv \gamma_1||x - x^*|| .$$

<u>Remark 2.1</u>. The theorem and proof are exactly the same if we replace L1 by L2 .

<u>Theorem 1</u>. Let x^* be a zero of $J_F^T(\cdot)F(\cdot)$ and let $K_i \geq 0$, be constants such that for every $x \in \Omega$
$||H_i(x) - H_i(x^*)|| \leq K_i||x - x^*||$ for each $i = 1,\ldots,M$.
Whenever $J_G(x^*)$ is non-singular, there exist constants $\delta > 0$, $\varepsilon > 0$ such that if $||x_o - x^*|| < \varepsilon$ and $||B_{i,o} - H_i(x_o)|| \leq \delta$, $i = 1,\ldots,M$, then algorithm 1.1 converges to x^* from x_o .

<u>Proof</u>. Choose C to be closure of a conditionally compact convex neighborhood of x^* . Furthermore, choose C sufficientl small so that J_G is invertible on C and $||J_G(x)^{-1}||$ is uniformly bounded by some constant B . Select a constant B' such that $||F(x)||_1$ is uniformly bounded on C by B' .

Let $K = \max_i K_i$ and pick $\delta < (6BB')^{-1}$ and $\varepsilon \leq \max\left(\frac{B'\delta}{\gamma_1}, \frac{\delta}{6K}\right)$ such that $N(x^*,\varepsilon) \subset C$. Now select $x_o, B_{1,o},\ldots,B_{M,o}$ as above. Set $A_o = \sum_{i=1}^{M} f_i(x_o)B_{i,o} + J_F(x_o)^T J_F(x_o)$.

$$||A_o - J_G(x_o)|| = ||\sum_{i=1}^{M} f_i(x_o)[B_{i,o} - H_i(x_o)]||$$

$$\leq \sum_{i=1}^{M} |f_i(x_o)| \cdot ||B_{i,o} - H_i(x_o)||$$

$$\leq ||F(x_o)||_1 \delta$$

$$\leq B'\delta .$$

Hence $||I - J_G(x_o)^{-1}A_o|| \leq BB'\delta < 1$ and so A_o^{-1} exists and is bounded in norm by $B(1 - BB'\delta)^{-1}$. Thus $x_1 = x_o - A_o^{-1}G(x_o)$ exists.

Set $e_1 = ||x_1 - x^*||$. Now

$$e_1 \leq ||A_o^{-1}|| \cdot [||G(x^*) - G(x_o) - A_o(x^* - x_o)||]$$

$$\leq ||A_o^{-1}|| \quad [||G(x^*) - G(x_o) - J_G(x_o)(x^* - x_o)|| + ||J_G(x_o) - A(x_o)||e_o]$$

$$\leq B(1 - BB'\delta)^{-1}[\gamma_1 e_o + ||F(x_o)||_1 \delta]\ e_o$$

$$\leq \frac{B\gamma_1 e_o + BB'\delta}{1-BB'\delta}\, e_o \leq \frac{2BB'\delta}{1-BB'\delta}\, e_o \leq \frac{2}{6} \cdot \frac{6}{5}\, e_o < \frac{1}{2}\, e_o .$$

Hence $J_G(x_1)$ and A_1 exist and as before:

$$||A_1 - J_G(x_1)|| \leq ||F(x_1)||_1 \max_i ||B_{i,1} - H_i(x_1)||$$

$$\leq B'[\ \delta + 2K(e_o + e_1)]$$

$$\leq B'(\delta + 3Ke_o) \leq B'\delta \cdot \frac{3}{2}$$

by Lemma 1. Thus, $||I - J_G(x_1)^{-1}A_1|| \leq BB'\delta \cdot 3/2 < 2BB'\delta < 1$. This means A_1^{-1} exists and is bounded in norm by $B(1 - 2BB'\delta)$, so x_2 exists.

Assume by way of induction that $x_1, \ldots, x_n$, $A_1^{-1}, \ldots, A_{n-1}^{-1}$ all exist and $e_k \leq \frac{1}{2} e_{k-1}$,

$\max_i ||B_{i,k} - H_i(x_k)|| \leq (2 - (\frac{1}{2})^k)\delta$, $k \leq n$. Then

$$||A_n - J_G(x_n)|| \leq ||F(x_n)||_1 \max_i ||B_{i,n} - H_i(x_n)|| \leq (2 - (\tfrac{1}{2})^n)B'\delta$$

and so $||I - J_G(x^n)^{-1}A_n|| < 2BB'\delta < \frac{1}{3}$. Hence A_n^{-1} exists and is bounded in norm by $B(1 - 2BB'\delta)^{-1}$, so x_{n+1} exists.

$$\begin{aligned} e_{n+1} &\leq ||A_n^{-1}|| \cdot [||G(x^*) - G(x_n) - J_G(x_n)(x_n - x^*)|| \\ &\qquad + ||J_G(x_n) - A_n||e_n] \\ &\leq ||A_n^{-1}|| \cdot [\gamma_1 e_n + (2 - (\tfrac{1}{2})^n)B'\delta]e_n \\ &\leq B(1 - 2BB'\delta)^{-1}[(\tfrac{1}{2})^n B'\delta + (2 - (\tfrac{1}{2})^n)B'\delta]e_n \\ &\leq 2BB'\delta(1 - 2BB'\delta)^{-1}e_n \\ &\leq \tfrac{1}{2} e_n . \end{aligned}$$

Now from Lemma 1,

$$\begin{aligned} ||B_{i,n+1} - H_i(x_{n+1})|| &\leq ||B_{i,n} - H_i(x_n)|| + 2K(e_n + e_{n+1}) \\ &\leq (2 - (\tfrac{1}{2})^n)\delta + 3Ke_n \\ &\leq [2 - (\tfrac{1}{2})^n + \tfrac{1}{2}(\tfrac{1}{2})^n]\delta \\ &= [2 - (\tfrac{1}{2})^{n+1}]\delta \end{aligned}$$

and the induction is complete. This implies that the sequence exists and $e_n \le (\frac{1}{2})^n e_0 \underset{n}{\to} 0$.

Theorem 2. If the hypotheses of Theorem 1 hold and $||F(x^*)|| = 0$, then the iteration defined by algorithm 1.1 converges at least quadratically.

Proof. $e_{n+1} \le B(1 - 2BB'\delta)^{-1}[\gamma_1 e_n^2 + ||F(x_n)||_1 (2 - (\frac{1}{2})^n)\delta e_n]$.

Now $||F(x_n)||_1 = ||F(x_n) - F(x^*)||_1 \le \max_{x \in C} ||J_F(x)|| e_n \equiv B'' e_n$.

Hence, $e_{n+1} \le B(1 - 2BB'\delta)^{-1}[\gamma_1 + 2B''\delta]e_n^2$.

Remark 2.1. If we assume the stronger continuity condition L2 for the H_i , namely

$$||H_i(x) - H_i(y)|| \le K_i ||x - y|| , \; i = 1,\ldots,M ,$$

then it is not necessary to assume the existence of a zero, x^* , of G : that is, by making assumptions about the behavior of the function and its derivatives in an open convex subset of E^N we are able to prove a "Kantorovich Theorem" [9] for the iteration defined by algorithm 1.1 in which the existence of x^* is deduced as a part of the proof.

3. Numerical Results.

Example 3.1. In order to test the method against a variety of algorithms in current use, we referred to the very fine survey paper by Box [2]. The test function used was

$$\phi(x_1,x_2,x_3) = \sum_p [e^{-x_1 p} - e^{-x_2 p}) - x_3(e^{-p} - e^{-10p})]^2$$

where the summation is over the values $p = 0.1(0.1)1.0$. This problem has a zero residual at $(1,10,1)$ and whenever $x_1 = x_2$ with $x_3 = 0$. We used those starting points for which $\phi(x^o)$ was large:

I. $x_1 = 0$, $x_2 = 10$, $x_3 = 20$ $\phi = 1031.154$

II. $x_1 = 0$, $x_2 = 20$, $x_3 = 20$ $\phi = 1021.655$

TABLE 1.

Number of Function Evaluations Required to Reduce ϕ to Less Than 10^{-5} (Example 3.1)

Method	Starting Point I	Starting Point II
Swann [17]	Failed	Failed
Rosenbrock [15]	350	246
Nelder and Mead [10] Spendley, Hext and Himsworth [16]	307	315
Powell (1964) [13]	Failed	Failed
Fletcher and Reeves [8]	92	188
Davidon [5] Fletcher and Powell [7]	140	140
Powell (1965) [14]	28	33
Barnes [1]	37	59
Algorithm 1.1 including evaluations done to approximate $H_1(x^o)$	37	33
Algorithm 1.1 when $H_1(x^o)$ was given approximately	24	20

Remark 3.1. Many of the methods above behave linearly and could not be expected to rapidly reduce ϕ from 10^{-5} to 10^{-10}; however, Algorithm 1.1 showed quadratic convergence in this range.

Example 3.2. This example is given by Nielsen [11] and is an illustration of how quadrature weights and nodes may be calculated by nonlinear least squares techniques.

Data Vectors:

p	y
0.0	2.0
1.0	0.0
2.0	2/3
3.0	0.0
4.0	2/5
5.0	0.0
6.0	2/7
7.0	0.0
8.0	2/9
9.0	0.0

Functional Relationship: $g(x;p) = x_1 x_3^p + x_2 x_4^p$.

Initial Approximation: $x_1 = 1.0$, $x_2 = 1.0$, $x_3 = -.75$, $x_4 = .75$

TABLE 2.

n	Gauss-Newton [11, p. 41]	$\phi(x^n)$	Algorithm 1.1	$\phi(x^n)$
1	.95493 .95493 -.68949 .68949	8.93674(-02)	.96373 .96301 -.69911 .69947	10.117(-02)
4	.97719 .97719 -.65194 .65194	7.46872(-02)	.97596 .97183 -.65219 .65047	.74687(-02
6	not reported		.97754 .97754 -.65140 .65140	.746847(-0
8	.97754 .97754 -.65140 .65140	7.46847(-02)	ten significant digits of accuracy	

Remark 3.2. The above example contrasts the slower convergence rate of the Gauss-Newton method with that of Algorithm 1.1, even in the presence of a small residual at the root.

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