On the Convergence of Broyden's Method for Nonlinear Systems of Equations

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Abstract. This paper uses majorant techniques to study the convergence of Broyden's single-rank update method for nonlinear systems of equations. It also contains a very elementary proof of the local convergence of the method. The heart of the method is a procedure for generating an approximation to the Jacobian of the system using only information on hand and not requiring partial derivatives.

1. Introduction. C. G. Broyden [2] suggested an algorithm for iterating to a solution of a system of nonlinear equations which has shown its mettle in dealing with practical problems. The purpose of this paper is to provide a Kantorovich-type analysis and an elementary local convergence proof for this method. In fact, the analysis is applicable to the entire class of 'single-rank update' methods just to the extent that it seems to justify heuristically the generally superior performance of Broyden's method over the rest of the class.

These methods generate sequences $\{x_n\}$, $\{H_n\}$, one consisting of approximate roots and the other of the corresponding approximate inverse Jacobian matrices. At the *n*th step, one obtains x_{n+1} from x_n and H_n by setting

(1)
$$x_{n+1} = x_n - \gamma_n H_n F(x_n),$$

where $F(x_n) = (f_1(x_n), \dots, f_n(x_n))^T$ is the residual vector at the point x_n , and γ_n is a real number about which more will be said later. H_{n+1} is obtained by using an idea due to Davidon [5]. It is required to satisfy the equation

(2)
$$H_{n+1}y_n \equiv H_{n+1}(F(x_{n+1}) - F(x_n)) = x_{n+1} - x_n.$$

This seems to be a very clever use of the small amount of new information furnished by $F(x_{n+1})$, since it is equivalent to

$$\int_{x_n}^{x_{n+1}} (H_{n+1}J(x) - I) \, dx = 0,$$

where J denotes the Jacobian matrix. It makes H_{n+1} look like a very reasonable approximation to the inverse Jacobian somewhere between x_n and x_{n+1} , at least in the direction $x_{n+1} - x_n$. For the single-rank methods, the choice of H_{n+1} from the class of $N \times N$ matrices satisfying (2) is

(3)
$$H_{n+1} = H_n - (H_n y_n + \gamma_n H_n F(x_n)) d_n^T / d_n^T y_n.$$

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If $B_i = H_i^{-1}$, then

$$B_{n+1} = B_n - (y_n + \gamma_n F(x_n)) d_n^T B_n / \gamma_n d_n^T F(x_n),$$

where $d_n \in E^n$ is, of course, chosen so that $d_n^T y_n \neq 0$.

Broyden [3] has shown that for his method, $d_n = H_n^T H_n F(x_n)$, if J(x) = L, a constant matrix, i.e., the system is linear, then $\{x_n\}$ and $\{H_n\}$ converge to x^* , the root, and L^{-1} , respectively, from any x_0 and any H_0 sufficiently close to L^{-1} .

Such a result would be too much to hope for when working with nonlinear systems, but in Section 2 we will show that the rate of deterioration in the approximation of $J(x_n)$ or $J(x^*)$ by B_n depends on the nonlinearity of F in a very simple way. This will enable us to analyze the method as a Newton-like method [7] in Section 3. In Section 4, we will draw some reasonable, though nonrigorous, conclusions, based on the results of Section 3, about the choice of γ . Any reader interested just in the local convergence can read only Lemma 3 and Theorem 5.

2. Error Bounds for the Jacobian Approximation. Let D_0 be an open convex set on which F is continuously differentiable. Let \bar{x} be a fixed element in D_0 and let K be a nonnegative number. We will always use the l_2 norm, so if A is a matrix, ||A|| is the square root of the spectral radius of $A^T A$. Remember that J is the function which maps x to the Jacobian of x.

Definition. $J \in \operatorname{Lip}_{\kappa} \{\bar{x}\}$ w.r.t. D_0 iff for every $x \in D_0$, $||J(x) - J(\bar{x})|| \leq K ||x - \bar{x}||$. $J \in \operatorname{Lip}_{\kappa} D_0$ if $J \in \operatorname{Lip}_{\kappa} \{x\}$ w.r.t. D_0 for every $x \in D_0$.

LEMMA 1. Let $J \in \text{Lip}_{\kappa} \{ \bar{x} \}$ w.r.t. D_0 , then for any $x \in D_0$,

$$||F(x) - F(\bar{x}) - J(\bar{x})(x - \bar{x})|| \leq (\frac{1}{2}K) ||x - \bar{x}||^2.$$

Proof. See [4] or [7]. LEMMA 2. Let $x, x' \in E^N$ with $x^T x' = 1$, then

$$||I - x'x^{T}|| = ||x'|| \cdot ||x||.$$

Proof. See [3].

LEMMA 3. Let x, $x' \in D_0$ and let B be an $N \times N$ real matrix. Let $d \in E^N$ with $d^T F(x) \neq 0$ and set

$$B' = B + (F(x') - F(x) - B(x' - x)) d^{T}B/d^{T}B(x' - x)$$

and

$$q \equiv \frac{||x' - x|| \cdot ||d^T B||}{|d^T B(x' - x)|}.$$

Under these conditions, if $J \in \text{Lip}_{\kappa} \{\bar{x}\}$ w.r.t. D_0 then

(4a)
$$||B' - J(\bar{x})|| \leq q||B - J(\bar{x})|| + \frac{qK}{2 \cdot ||x' - x||} (||x' - \bar{x}||^2 + ||x - \bar{x}||^2).$$

If $J \in \operatorname{Lip}_{\kappa} D_0$, then

(4b)
$$||B' - J(x')|| \leq q||B - J(x)|| + K(1 + \frac{1}{2}q) ||x' - x||.$$

Proof. Assume that we have established (4a); then, since $J \in \text{Lip}_{\pi} D_0$, we can set $\bar{x} = x$ and add ||J(x) - J(x')|| to both sides of (4a) to obtain (4b). (4a) is easily seen

(3')

to follow from the following indentities.

$$B' - J(\bar{x}) = B - J(\bar{x}) + (F(x') - F(\bar{x}) - J(\bar{x})(x' - \bar{x})) \frac{d^{T}B}{d^{T}B(x' - x)}$$
$$- (F(x) - F(\bar{x}) - J(\bar{x})(x - \bar{x})) \frac{d^{T}B}{d^{T}B(x' - x)}$$
$$- (B - J(\bar{x}))(x' - x) \frac{d^{T}B}{d^{T}B(x' - x)}.$$

Now, apply Lemma 1 to the two middle terms and Lemma 2 to the combination of the first and last terms.

We will now apply (4b) to the case when $B = B_n$, $B' = B_{n+1}$, $x = x_n$, $x' = x_{n+1}$, $d = d_n$. In the next theorem, interpret the quotient q_n in the obvious way and define $q_{-1} \equiv 1$.

THEOREM 1. Let $J \in \text{Lip}_K D_0$ and let $x_0, \dots, x_{n+1}, B_0, \dots, B_{n+1}$ be generated by any single-rank method. If $\{x_i : i = 1, \dots, n+1\} \subset D_0$, then

(5)
$$||B_{n+1} - J(x_{n+1})|| \leq \left(\prod_{j=0}^{n} q_{j}\right) ||B_{0} - J(x_{0})|| + K \sum_{j=0}^{n} \left(\prod_{i=-1}^{n-j-1} q_{i}\right) (1 + \frac{1}{2}q_{i}) ||x_{j+1} - x_{j}||$$

Proof. The proof will be by induction on n + 1.

Let n + 1 = 1. By making the proper substitutions in (4b),

$$||B_1 - J(x_1)|| \leq q_0||B_0 - J(x_0)|| + K(1 + \frac{1}{2}q_0)||x_1 - x_0||,$$

which is (5) for n = 0. Assume by way of induction that (5) holds for $n + 1 \le k$. Then, again by (4),

$$\begin{aligned} ||B_{k} - J(x_{k})|| \\ \leq \left(\prod_{i=0}^{k-1} q_{i}\right) ||B_{0} - J(x_{0})|| + K \sum_{i=0}^{k-1} \left(\prod_{i=-1}^{k-1-i-1} q_{i}\right) (1 + \frac{1}{2}q_{i}) ||x_{i+1} - x_{i}||, \end{aligned}$$

and so

$$||B_{k+1} - J(x_{k+1})||$$

$$\leq q_k \left[\left(\prod_{i=0}^{k-1} q_i \right) ||B_0 - J(x_0)|| + K \sum_{i=0}^{k-1} \left(\prod_{i=-1}^{k-1-i-1} q_i \right) (1 + \frac{1}{2}q_i) ||x_{i+1} - x_i|| \right]$$

$$+ K(1 - \frac{1}{2}q_k) ||x_{k+1} - x_k||$$

$$= (5)$$

with n + 1 = k + 1 and the induction is complete.

Now, obviously, $q_n \ge 1$ and, just as obviously, any analysis based on (5) needs $q_n = 1$ or that $\prod q_i$ is uniformly bounded. There are various ways of 'fudging' however in order to control the deterioration [1], [6].

The Cauchy inequality tells us that $q_n = 1$ if and only if there is a constant $c_n \neq 0$ such that $B_n^T d_n = c_n(x_{n+1} - x_n) = c'_n H_n F_n$, i.e., $d_n = c'_n H_n^T H_n F_n$, Broyden's choice. If we view a particular method as the selection function for d_n , then a glance at (3) and (3') convinces us that the two methods are the same if $d'_n = c_n d_n$ for some sequence $\{c_n\}$ of nonzero constants. Hence, Broyden's method is the unique single-rank method which is naturally of bounded deterioration. It seems unnecessary to find the general analogue of (5) for (4a). The analogue for Broyden's method is the heart of the proof of Theorem 5.

3. A Kantorovich-Type Analysis for Broyden's Method. In [7], the author considers the convergence of a class of Newton-like methods of the form

(6)
$$x_{n+1} = x_n - A(x_n)^{-1}F(x_n).$$

An immediate corollary of the results there is the following important extension of Rheinboldt's Theorem [10].

THEOREM 2. Let F be as above and let A have the property that given any $x \in D_0$, A(x) is an $N \times N$ real matrix. Let δ_0 , δ_1 be nonnegative real numbers such that

(7)
$$||A(x) - J(x)|| \leq \delta_0 + \delta_1 ||x - x_0||$$

for every $x \in D_0$ and let β and η be real numbers such that $A(x_0)^{-1}$ exists and $||A(x_0)^{-1}|| \leq \beta$, $||A(x_0)^{-1}F(x_0)|| \leq \eta$.

Then, $1 > \beta \delta_0, \frac{1}{2} \ge h' \equiv \beta K \eta / (1 - \beta \delta_0)^2$ and $N(x_0, r'_0) \subset D_0$, where

$$r'_{0} \equiv \frac{1 - (1 - 2h')^{1/2}}{\beta K} (1 - \beta \delta_{0}),$$

imply that F has a root $x^* \in \overline{N}(x_0, r'_0)$ which is unique in $D_0 \cap N(x_0, r_1)$, where

$$r_1 \equiv \frac{1 + (1 - 2h')^{1/2}}{\beta K} (1 - \beta \delta_0).$$

Furthermore, $x'_{n+1} = x'_n - A(x_0)^{-1}F(x'_n)$ converges to x^* from any $x'_0 \in D_0 \cap N(x_0, r_1)$.

If in addition, $1 > 3\beta \delta_0$, $\frac{1}{2} \ge h \equiv (2\delta_1 + K)\beta \eta/(1 - 3\beta \delta_0)^2$ and $N(x_0, r_0) \subset D_0$, where

$$r_0 \equiv \frac{1 - (1 - 2h)^{1/2}}{\beta(2\delta_1 + K)} (1 - 3\beta\delta_0),$$

then the sequence $\{x_n\}$ generated by (6) converges to x^* .

The fact that the theorem ensures convergence of the $\{x'_n\}$ sequence under less stringent conditions than for the $\{x_n\}$ sequence is a characteristic of this type of theorem and results from using the $\{x'_n\}$ sequence to establish the existence and uniqueness of x^* .

If we write (5) for the special case of Broyden's method, we obtain

(5')
$$||B_{n+1} - J(x_{n+1})|| \leq ||B_0 - J(x_0)|| + \frac{3K}{2} \sum_{j=0}^n ||x_{j+1} - x_j||$$

which, except for a wrong-way triangle inequality, looks like a version of (7) with $\delta_0 = ||B_0 - J(x_0)||$, $\delta_1 = \frac{3}{2}K$ and the function A only defined at the iteration points. One is immediately led to conjecture the following theorem for Broyden's method.

THEOREM 3. Let $F \in \text{Lip}_{\kappa} D_0$ and let B_0 be a nonsingular $N \times N$ matrix such

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that $||J(x_0) - B_0|| \leq \delta$, $||H_0|| \leq \beta$ and $||H_0F(x_0)|| \leq \eta$. Then, $1 > \beta\delta$, $\frac{1}{2} \geq h = \beta K/(1 - \beta\delta)^2$ and $N(x_0, r'_0) \subset D_0$, where

$$r'_{0} = \frac{1 - (1 - 2h')^{1/2}}{\beta K} (1 - \beta \delta)$$

imply that F has a root x^* , $||x_0 - x^*|| \leq r'_0$, and x^* is unique in $D_0 \cap N(x_0, r'_1)$, where

$$r'_{1} = \frac{1 + (1 - 2h')^{1/2}}{\beta K} (1 - \beta \delta).$$

Furthermore, $x'_{n+1} = x'_n - H_0 F(x'_n)$ converges to x^* from any $x'_0 \in D_0 \cap N(x_0, r'_1)$. If in addition, $1 > 3\beta\delta, \frac{1}{8} \ge h \equiv \beta K \eta / (1 - 3\beta\delta)^2$ and $N(x_0, r_0) \subset D_0$, where

$$r_0 \equiv \frac{1 - (1 - 8h)^{1/2}}{4\beta K} (1 - 3\beta \delta),$$

then Broyden's method with $\gamma_n = 1$ for every n, converges to x^* .

The existence and uniqueness of x^* and the convergence of the x' sequence can be obtained directly from Theorem 2 by, for example, setting $A(x) \equiv B_0$ for every $x \in D_0$. Thus, we make the second set of assumptions and proceed to a consideration of the full Broyden sequence. The first step in the proof of Theorem 2 by the techniques of [7] is to show that A(x) is always invertible and to find a scalar function $a(\cdot)$ such that $a(||x - x_0||)^{-1} \ge ||A(x)^{-1}||$ for every $x \in N(x_0, r_0)$. Let us assume that, for $n \ge 0$, $\sum_{i=0}^{n} ||x_{i+1} - x_i|| < r_0$. Then from (5'),

$$\begin{aligned} ||H_0B_{n+1} - I|| &\leq \beta ||B_{n+1} - B_0|| \\ &\leq \beta[||B_{n+1} - J(x_{n+1})|| + ||J(x_{n+1}) - J(x_0)|| + ||J(x_0) - B_0||] \\ &\leq \beta \left(2\delta + \frac{3K}{2} \sum_{i=0}^n ||x_{i+1} - x_i|| + K||x_{n+1} - x_0|| \right) \\ &\leq 2\beta\delta + \frac{5\beta K}{2} \sum_{i=0}^n ||x_{i+1} - x_i|| < 2\beta\delta + \frac{5}{2}\beta Kr_0 \\ &= 2\beta\delta + \frac{5}{8}(1 - (1 - 8h)^{1/2})(1 - 3\beta\delta) \leq 3\beta\delta + c(1 - 3\beta\delta) < 1 \end{aligned}$$

since c < 1. Hence, by the Banach Lemma [7], [8], $(H_0 B_{n+1})^{-1} H_0 = H_{n+1}$ exists and is bounded in norm by $\beta(1 - 2\beta\delta - (5\beta K/2)\sum_{i=0}^{n} ||x_{i+1} - x_i||)^{-1}$.

Let $b_0 = \beta^{-1}$ and $h_0 = \beta$, $t_0 = 0$. Define $f(t) = 2Kt^2 - (b_0 - 3\delta)t + b_0\eta$, $h_k = \beta(1 - 2\beta\delta - 5\beta Kt_k/2)^{-1}$, $h_k^{-1} = b_k$ and consider the sequence $t_{k+1} = t_k + h_k f(t_k)$. Notice that $r_0 > t_1 = \eta \ge ||H_0F(x_0)|| = ||x_1 - x_0||$. Suppose now that $0 < t_k < r_0$, then, since $f(r_0) = 0$, $r_0 - t_{k+1} = r_0 - t_k + h_k(f(r_0) - f(t_k)) = (r_0 - t_k)(1 + h_k f'(\xi))$, $\xi \in (t_k, r_0)$. Now,

$$f'(\xi) = 4K\xi - (b_0 - 3\delta) < 4Kr_0 - (b_0 - 3\delta)$$

= $(1 - (1 - 8h)^{1/2})(b_0 - 3\delta) - (b_0 - 3\delta) = -(1 - 8h)^{1/2} \cdot (b_0 - 3\delta) < 0.$

Hence, $1 + h_k f'(\xi) < 1$ so $r_0 - t_{k+1} < r_0 - t_k$. Furthermore, $h_k \ge \beta = h_0$, so $h_k f'(\xi) \ge -h_0(b_0 - 3\delta) = -1 + 3\beta\delta > -1$ and $1 + h_k f'(\xi) > 0$. Thus, $0 < r_0 - t_{k+1} < r_0 - t_k$ and $\{t_k\}$ is a strictly increasing sequence in $[0, r_0]$. Hence, it converges to $t^* \le r_0$. If $t^* < r_0$, then $t^* = t^* + \beta(1 - 2\beta\delta - 5K\beta t^*/2)^{-1} f(t^*)$, and

so $f(t^*) = 0$. This ensures that $t^* = r_0$, since r_0 is the smallest root of f in $[0, r_0]$. We have already that $t_1 \ge ||x_1 - x_0||$. Suppose now that x_0, x_1, \dots, x_k satisfy the properties that $||x_{i+1} - x_i|| \le t_{i+1} - t_i$, $i = 0, 1, \dots, k - 1$. Then $\sum_{i=0}^{k-1} ||x_{i+1} - x_i|| \le t_k < r_0$ and H_k exists with $||H_k|| \le h_k$. Now, apply Lemma 1 and (5'):

$$\begin{aligned} ||x_{k+1} - x_k|| \\ &\leq h_k[||F(x_k) - F(x_{k-1}) - J(x_{k-1})(x_k - x_{k-1})|| + ||J(x_{k-1}) - B_{k-1}|| \cdot ||x_k - x_{k-1}||] \\ &\leq h_k \bigg[\frac{1}{2}K||x_k - x_{k-1}||^2 + \bigg(\delta + \frac{3}{2}K \sum_{j=0}^{k-2} ||x_{j+1} - x_j|| \bigg) ||x_k - x_{k-1}|| \bigg] \\ &\leq h_k [\frac{1}{2}K(t_k - t_{k-1})^2 + (\delta + \frac{3}{2}Kt_{k-1})(t_k - t_{k-1})] \frac{f(t_{k-1})}{t_k - t_{k-1}} + f'(t_{k-1}) \\ &= b_{k-1} + f'(t_{k-1}) \\ &= b_0(1 - 2h_0\delta - \frac{5}{2}\beta Kt_{k-1}) + \frac{4Kt_{k-1}}{2} - (b_0 - 3\delta) \\ &= b_0 - 2\delta - \frac{5}{2}\beta b_0 Kt_{k-1} + 4Kt_{k-1} - b_0 + 3\delta = \delta + \frac{3}{2}Kt_{k-1}. \end{aligned}$$

We can thus write

$$||x_{k+1} - x_k|| \leq h_k [2K(t_k - t_{k-1})^2 + f'(t_{k-1})(t_k - t_{k-1}) + f(t_{k-1})]$$
$$\leq h_k f(t_k) = t_{k+1} - t_k,$$

since the bracketed expression is the Taylor expansion for the quadratic f. Now, we can conclude by induction that $\sum_{i=0}^{k} ||x_{i+1} - x_i|| \leq t_k < r_0$ for every k. Hence, $\{x_n\}$ is a Cauchy sequence and must converge to some $x^{**} \in \overline{N}(x_0, r_0)$. It only remains for us to show that $x^{**} = x^*$. From (5'), we obtain $||B_k|| \leq ||J(x_k)|| + \delta + \frac{3}{2}Kt_k \leq ||J(x_0)|| + \delta + 5Kt_k/2 < ||J(x_0)|| + \delta + 5Kr_0/2 \equiv C$. Hence

$$||F(x^{**})|| = \lim_{k} ||F(x_{k})|| = \lim_{k} ||B_{k}|| \cdot ||x_{k+1} - x_{k}|| \leq C \lim_{k} ||x_{k+1} - x_{k}|| = 0.$$

Now, $r_0 < r'_1$ so the unicity assertion concerning x^* ensures that $x^* = x^{**}$. The following corollary is straightforward.

THEOREM 4. Let x^* be a root of the nonlinear system F. Let the first partial derivatives satisfy a Lipschitz condition of order 1 in some open set containing x^* and let $J(x^*)$ be invertible. Under these conditions, there is an $\epsilon > 0$ and a $\delta > 0$ such that if x_0 is any N-vector and B_0 is any matrix satisfying $||x_0 - x^*|| < \epsilon$ and $||J(x_0) - B_0|| < \delta$, then Broyden's method with $\gamma_n = 1$ for all n converges to x^* from x_0 .

It is possible to give a more elementary proof of local convergence which requires only that $J \in \text{Lip}_{K} \{x^*\}$ w.r.t. D_0 . This condition holds for example if all the first partials of F exist around x^* and the difference quotients of the first partials are bounded at x^* . This is the continuity condition often used to provide a simple proof of the local quadratic convergence of Newton's method.

THEOREM 5. Let x^* be a root of F and $J \in \text{Lip}_{\kappa} \{x^*\}$ w.r.t. D_0 . Under these conditions, if $J(x^*)$ is invertible, then there exist real positive numbers ϵ and δ such that if B_0 is a real $N \times N$ matrix, $||B_0 - J(x^*)|| \leq \delta$, and $||x_0 - x^*|| < \epsilon$, Broyden's method with $\gamma_n \equiv 1$ converges to x^* from this starting point.

Proof. Let β bound $||J(x^*)^{-1}||$. Choose $\delta \leq 1/6B$ and $\epsilon \leq 2\delta/5K$, such that $N(x_0, \epsilon) \subset \Omega_0$. Now, select x_0, B_0 as above. It is clear from the Banach Lemma [7], [8]

that H_0 exists and is bounded in norm by $\beta(1 - \beta \delta)^{-1}$. The choice of ϵ ensures that $F(x_0)$ exists and so x_1 exists.

$$e_{1} \equiv ||x_{1} - x^{*}|| = ||x_{0} - x^{*} - H_{0}(F(x_{0}) + F(x^{*}))||$$

$$\leq ||-H_{0}|| \cdot ||F(x_{0}) - F(x^{*}) - B_{0}(x_{0} - x^{*})||$$

$$\leq ||H_{0}|| [||F(x_{0}) - F(x^{*}) - J(x^{*})(x_{0} - x^{*})|| + ||J(x^{*}) - B_{0}|| \cdot ||x_{0} - x^{*}||]$$

$$< \frac{\beta}{1 - \beta\delta} \left(\frac{1}{2}Ke_{0}^{2} + \delta e_{0}\right) \leq \frac{\beta}{1 - \beta\delta} \left(\frac{1}{2}Ke_{0} + \delta\right)e_{0}$$

$$\leq \frac{\beta}{1 - \beta\delta} \left(\frac{\delta}{5} + \delta\right)e_{0} \leq \frac{\delta}{5} \frac{\beta\delta}{1 - \beta\delta}e_{0} < \frac{1}{2}e_{0}.$$

Hence, $F(x_1)$ and B_1 exist. Now,

$$||x_1 - x_0|| \ge ||x_0 - x^*|| - ||x_1 - x^*|| \ge e_0 - \frac{1}{2}e_0 = \frac{1}{2}e_0.$$

Applying Lemma 3 and the above, we obtain

$$||B_1 - J(x^*)|| \leq \delta + \frac{K}{2} \left(\frac{1}{4}e_0^2 + e_0^2\right) ||x_1 - x_0||^{-1}$$
$$\leq \delta + \frac{5}{4} Ke_0 \cdot \frac{1}{2}e_0 ||x_1 - x_0||^{-1}$$
$$\leq \delta + \frac{5}{4} Ke_0 \leq \frac{3}{2} \delta < 2\delta.$$

Hence, $||J(x^*)^{-1}B_1 - I|| < 2\beta\delta$, so H_1 exists and is bounded in norm by $\beta(1 - 2\beta\delta)^{-1}$, so x_2 is defined. Assume by way of induction that $x_1, \dots, x_n, H_1, \dots, H_{n-1}$ all exist and $e_k \leq \frac{1}{2}e_{k-1}$, $||B_k - J(x^*)|| \leq (2 - (\frac{1}{2})^k)\delta$, $k \leq n$. Then, $||J(x^*)^{-1}B_n - I|| \leq (2 - (\frac{1}{2})^k\beta\delta < \frac{1}{3}$ and so H_n exists by the Banach Lemma and is bounded in norm by $\beta(1 - 2\beta\delta)^{-1}$. This ensures that x_{n+1} exists. Now

$$e_{n+1} \leq ||H_n|| \cdot [||F(x_n) - F(x^*) - J(x^*)(x_n - x^*)|| + ||J(x^*) - B_n||e_n]$$

$$\leq \beta (1 - 2\beta \delta)^{-1} [\frac{1}{2} K e_n^2 + (2 - (\frac{1}{2})^n) \delta e_n]$$

$$\leq \beta (1 - 2\beta \delta)^{-1} [(\frac{1}{2})^n (\delta/5) + (2 - (\frac{1}{2})^n) \delta] e_n$$

$$< \beta (1 - 2\beta \delta)^{-1} 2 \delta e_n < \frac{1}{2} e_n.$$

We complete the induction by applying Lemma 3 to write

$$||B_{n+1} - J(x^*)|| \leq ||B_n - J(x^*)|| + \frac{1}{2}K(e_{n+1}^2 + e_n^2) ||x_{n+1} - x_n||^{-1}$$

$$\leq (2 - (\frac{1}{2})^n)\delta + \frac{5}{4}Ke_n$$

$$\leq (2 - (\frac{1}{2})^n + \frac{5}{4} \cdot (\frac{1}{2})^n \cdot \frac{2}{5})\delta$$

$$= (2 - (\frac{1}{2})^n + (\frac{1}{2})^{n+1})\delta$$

$$= (2 - (\frac{1}{2})^{n+1})\delta.$$

We have used here that, as above, $\frac{1}{2}e_n \leq ||x_{n+1} - x_n||$.

Hence, the sequence $\{x_n\}$, $\{H_n\}$ exists and $e_n \leq (\frac{1}{2})^n e_0$, so Broyden's method converges.

In Lemma 3 and the theorem above, we note that if K = 0, i.e., the system is linear, then $||B_n - J(x^*)|| \leq ||B_0 - J(x^*)||$ and $\epsilon = \infty$. This is simply a reflection of the fact, indicated by the expression for e_1 in terms of e_0 , that for a linear system, $\delta \leq 1/2\beta$ is sufficient to ensure convergence from any x_0 . See [3].

It is simple to change the hypothesis of Theorem 5 so that B_0 is required to be close to $J(x_0)$ instead of $J(x^*)$.

COROLLARY 5. Under the hypothesis of Theorem 5, there exist real positive numbers δ' , ϵ' such that if $||x_0 - x^*|| \leq \epsilon'$, and B_0 is a real $N \times N$ matrix, $||B_0 - J(x_0)|| \leq \delta'$, then Broyden's method converges to x^* from this starting point.

Proof. Let ϵ and δ be as in the previous theorem. Select $\epsilon' \leq \epsilon$ and δ' such that $\delta' + K\epsilon' \leq \delta$. Now, let $||x_0 - x^*|| < \epsilon'$, $||B_0 - J(x_0)|| < \delta'$. Then, $||B_0 - J(x^*)|| \leq ||B_0 - J(x_0)|| + ||J(x_0) - J(x^*)|| \leq \delta' + K\epsilon' \leq \delta$ and $||x_0 - x^*|| < \epsilon$, so the result follows from Theorem 5.

4. The Choice of γ_n . In the introduction, we made the obvious statement that d_n was chosen so that $d_n^T y_n \neq 0$. Clearly, this requirement alone allows us to define H_{n+1} from H_n by (3). The following theorem clarifies this requirement.

THEOREM 6. Let H_n be a nonsingular $N \times N$ matrix and let $d_n \in E^N$, such that $d_n^T y_n \neq 0$. Then, H_{n+1} is nonsingular if and only if $d_n^T F(x_n) \neq 0$.

Proof. First, let us assume that $d_n^T F(x_n) = 0$. Direct substitution in (3) yields $H_{n+1}F(x_n) = H_nF(x_n)$. Also,

$$H_{n+1}F(x_{n+1}) = H_nF(x_{n+1}) - (H_ny_n + \gamma_nH_nF(x_n))\frac{d_n^TF(x_{n+1})}{d_n^Ty_n}$$

= $H_nF(x_{n+1}) - H_ny_n - \gamma_nH_nF(x_n) = (1 - \gamma_n)H_nF(x_n)$

If $\gamma_n = 1$, H_{n+1} is clearly singular. If $\gamma_n \neq 1$, then as above, $H_{n+1}F(x_{n+1}) = (1 - \gamma_n)H_{n+1}F(x_n)$ and so $H_{n+1}(F(x_{n+1}) - (1 - \gamma_n)F(x_n)) = 0$. Hence, either H_{n+1} is singular or $F(x_{n+1}) = (1 - \gamma_n)F(x_n)$. If the latter were true, then $d_n^T F(x_{n+1}) = 0$ and $d_n^T y_n = 0$ would result. This would contradict the hypothesis $d_n^T y_n \neq 0$, so H_{n+1} is singular.

Assume now that $H_{n+1}x = 0$ for some $x \neq 0$. Clearly, $d_n^T x \neq 0$ since H_{n+1} agrees with the nonsingular matrix H_n on the orthogonal complement of d_n . From (3),

$$H_n x = (H_n y_n + \gamma_n H_n F(x_n)) d_n^T x / d_n^T y_n$$

and so

$$x = (y_n + \gamma_n F(x_n)) d_n^T x / d_n^T y_n.$$

Hence, $d_n^T x = (d_n^T y_n + \gamma_n d_n^T F(x_n)) d_n^T x/d_n^T y_n$ and so $\gamma_n d_n^T F(x_n) = 0$. Now, if $\gamma_n = 0$, $F(x_{n+1}) = F(x_n)$ and $d_n^T y_n = 0$, so we can conclude that d_n is perpendicular to $F(x_n)$. The previous theorem obviously has a more general analogue in the language of

Lemma 3. The proof of Theorem 6 could have been simplified by using (3') but we wanted

The proof of Theorem 6 could have been simplified by using (3') but we wanted the little result that $d_n^T F(x_n) = 0$ implies $H_{n+1}F(x_{n+1}) = (1 - \gamma_n)H_nF(x_n)$.

Let us suppose that we are choosing γ_n by some minimization criterion like $\min_{\gamma} ||F(x_n - \gamma H_n F(x_n))||$. In a difficult situation, we may have to settle for a small γ_n and $F(x_{n+1})$ close to $F(x_n)$. This means that y_n is close to zero and, since the norm

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of d_n is relatively irrelevant, $d_n^T y_n$ would be close to zero. The obvious remedy is to set $d_n = y_n$. Now, we note that $d_n^T F(x_n) = F(x_{n+1})^T F(x_n) - F(x_n)^T F(x_n)$ will be near zero and so the new direction of search $H_{n+1}F(x_{n+1}) \approx H_nF(x_n)$, the direction we have just searched unsuccessfully. C. G. Broyden confirms that the above heuristics fit his computational experience with $d_n = y_n$. See [2].

In Broyden's successful method, also defined in [2], $d_n = -H_n^T H_n F(x_n)$ and so $d_n^T F(x_n)$ is in no serious danger of going to zero except as a result of convergence, i.e., the direction of search will probably not suffer too much from a small γ_n . Of course, $d_n^T y_n$ will be in danger and so the magnitude of the correction will be distorted and it may be desirable to obtain a fresh approximate Jacobian. This seems to explain behavior observed by M. J. D. Powell [9].

A useful strategy for choosing γ would probably be based on the one outlined by A. Goldstein [8] for Newton's method. It would seem reasonable to choose γ by some descent criterion until one feels he has a good approximate root and then switch to $\gamma \equiv 1$.

5. Concluding Remarks. In this investigation we have ignored the fact that for many problems the direction d_n will sweep through a basis often enough to make (5) and (5') unduly pessimistic. Powell [9], at additional computational expense, modifies Broyden's correction in such a way that B_n converges to $J(x^*)$ if x_n converges to x^* . There seems little doubt that Powell's modification is justified for many problems.

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