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The Convergence of Quasi-Gauss-Newton Methods for Nonlinear Problems

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Abstract—Quasi-Gauss-Newton methods for nonlinear equations are investigated. A Quasi-Gauss-Newton method is proposed. In this method, the Jacobian is modified by a convex combination of Broyden's update and a weighted update. The convergence of the method described by Wang and Tewarson in [1] and the proposed method is proved. Computational evidence is given in support of the relative efficiency of the proposed method.

1. INTRODUCTION

In this paper, we consider methods for finding a solution, x^* say, to a nonlinear system of algebraic equations

$$f(x) = 0, (1)$$

where the function $f: \mathbb{R}^n \to \mathbb{R}^n$ is nonlinear in $x \in \mathbb{R}^n$.

The classical method to determine x^* for (1) is the Newton method, which approximates f_i , i = 1, ..., n, by a linear function. Thus,

$$f(x+s) = f(x) + J(x)s + O(||s||^2)$$

where J(x) is the Jacobian at x. The next iterate can be obtained from the solution of

$$J(x)s = -f(x),$$

or, equivalently, by solving the normal equation

$$J(x)^{\top}J(x)s = -J(x)^{\top}f(x)$$
⁽²⁾

for s. It is evident that s is the solution of the linear least-square problem

minimize
$$\frac{1}{2} \|f(x+s)\|_2^2$$
.

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Equation (2) is usually computed by QR decomposition of J(x). If B is an approximation to J(x), then (2) can be replaced by

$$B^{\mathsf{T}}Bs = -B^{\mathsf{T}}f(x). \tag{3}$$

One well-known approximation for J(x) is by updating the initial Jacobian at each step with Broyden's update. It has been shown in [1] that using LDL^{\top} factorization of $B^{\top}B$ leads to more superior computational results than the so-called SQRT method for a given set of test problems. It is also shown that, if the modified Cholesky factorization in [2] is used, the number of operations is reduced from $O(n^3)$ to $O(n^2) + n$. In this paper, a convex combination of Broyden's update and a weighted update is used for the Jacobian approximation B in (3) instead of Broyden's update. This leads to a better convergence rate. We now describe Broyden's update and its convex combination with another update.

Jacobian Approximations

Solving the systems of nonlinear equations (1) involves the computation of the Jacobian. It is known that the computation of the Jacobian is expensive, especially when functions are difficult to evaluate. The Jacobian approximations have been widely used to save time. One of the most successful approximations is known as Broyden's update [3,4].

Using linearization, we have

$$0 = f(x^*) = f(x + x^* - x) \approx f(x) + J(x)(x^* - x)$$

Let x_k be an approximation to x^* , $B_k \approx$ the Jacobian at the k^{th} step and $x^* = x_k + s$. Then the k^{th} step is

$$0 = f(x_k) + J(x_k)(x^* - x_k)$$
$$= f(x_k) + J(x_k) s$$
$$\approx f(x_k) + B_k s.$$

At the $(k+1)^{\text{th}}$ step,

 $x^* \approx x_{k+1} = x_k + s$

or

$$x_{k} = x_{k+1} - s$$

$$f(x_{k}) = f(x_{k+1}) - J(x_{k+1}) s \approx f(x_{k+1}) - B_{k+1}s$$

Since $B_{k+1}s$ can be written as $(B_k + \Delta B)s$, from the last equation, we have

$$\Delta Bs = f(x_{k+1}). \tag{4}$$

 ΔB has been determined in many ways. One of them is Broyden's update,

$$\Delta B_1 = \frac{f(x_{k+1}) \, s^{\mathsf{T}}}{s^{\mathsf{T}} s}.$$
(5)

Since $-B^{\top}f(x)$ in (3) is the steepest descent direction computed at each iteration, we will utilize this information in approximating the Jacobian to get a better estimate. A solution of (4) is

$$\Delta B_2 = f\left(x_{k+1}\right) \frac{s^\top B^\top B}{s^\top B^\top B s} = f\left(x_{k+1}\right) \frac{t^\top}{s^\top t},$$

where $t = -B^{\top}f$.

We now combine two updates to approximate the update ΔB to the Jacobian. It was shown in [5] that this leads to a better update. The convex combination of the updates is

$$\Delta B = (1 - \mu)\Delta B_1 + \mu\Delta B_2 \tag{6}$$

where μ is chosen from

$$\|\Delta B_1\|_F = \frac{\|\Delta B_1\|_F}{\|\Delta B_2\|_F} \|\Delta B_2\|_F = \mu \|\Delta B_2\|_F,$$

therefore, $\mu = \frac{(s^{\top}t)^2}{s^{\top}st^{\top}t}$.

Next, we describe how the equation (3) can be solved effectively when the update is given by (5).

2. QUASI-GAUSS-NEWTON METHODS

In this section, we describe how the LDL^{\top} factorization in [2] can be utilized for solving (3) with the Jacobian approximation given in the previous section.

The method uses an algorithm in [2], which is for a symmetric matrix A modified by a symmetric matrix of rank one,

$$\overline{A} = A + \alpha z z^{\top} \tag{7}$$

and finds the Cholesky factors of $\overline{A} = \overline{LDL}^{\top}$ from the factors of $A = LDL^{\top}$. If A is replaced by $B^{\top}B$ in (7) and $B^{\top}B$ is modified by a rank one update, then

$$\overline{B}^{\mathsf{T}}\overline{B} = B^{\mathsf{T}}B + \alpha z z^{\mathsf{T}} = L \left(D + \alpha p p^{\mathsf{T}} \right) L^{\mathsf{T}},\tag{8}$$

where Lp = z, and p is obtained from z. If we factor

$$D + \alpha p p^{\top} = \tilde{L} \tilde{D} \tilde{L}^{\top},$$

the required modified Cholesky factors are of the form,

$$\overline{B}^{\top}\overline{B} = L\tilde{L}\tilde{D}\tilde{L}^{\top}L^{\top}$$

Therefore,

$$\overline{L} = L\tilde{L}, \overline{D} = \tilde{D}.$$

Initially, the orthogonal factorization of B is such that $B^{\top}B = R^{\top}R$ and initial L and D can be obtained from $R^{\top}R$. The algorithm for updating L and D is: ALGORITHM 2.1.

Define
$$\alpha_1 = \alpha, w^{(1)} = z.$$

Do for $j = 1, \dots n:$
 $p_j = w_j^{(j)},$
 $\overline{d}_j = d_j + \alpha_j p_j^2,$
 $\beta_j = p_j \frac{\alpha_j}{\overline{d}_j},$
 $\alpha_{j+1} = d_j \frac{\alpha_j}{\overline{d}_j}$
Do for $r = j + 1, \dots, n.$
 $w_r^{(j+1)} = w_r^{(j)} - p_j l_{rj}$
 $\overline{l}_{rj} = l_{rj} + \beta_j w_r^{(j+1)}$

If $\overline{B} = B + \frac{\overline{f}s^{\mathsf{T}}}{s^{\mathsf{T}}s}$ is used in (8),

$$\overline{B}^{\mathsf{T}}\overline{B} = B^{\mathsf{T}}B + B^{\mathsf{T}}\frac{\overline{f}s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \frac{s\overline{f}^{\mathsf{T}}}{s^{\mathsf{T}}s}B + \frac{s\overline{f}^{\mathsf{T}}}{s^{\mathsf{T}}s}\frac{\overline{f}s^{\mathsf{T}}}{s^{\mathsf{T}}s}.$$
(9)

From the above equation, we can see that $B^{\top}B$ is modified by a rank-2 update and (9) can be rewritten as

$$\overline{B}^{\mathsf{T}}\overline{B} = B^{\mathsf{T}}B + z_1 z_1^{\mathsf{T}} - z_2 z_2^{\mathsf{T}}$$

where

$$z_1 = \frac{\overline{B}^\top \overline{f} + \left(1 - \overline{f}^\top \overline{f}/2\right) \frac{s^\top}{s^\top s}}{\sqrt{2}}$$

and

$$z_2 = rac{\overline{B}^{ op}\overline{f} - \left(1 + \overline{f}^{ op}\overline{f}/2
ight)rac{s^{ op}}{s^{ op}s}}{\sqrt{2}}.$$

The algorithm for Quasi-Gauss-Newton method [1] using Broyden's update is as follows. ALGORITHM 2.2.

Given
$$f: \mathbb{R}^n \to \mathbb{R}^n, x_0 \in \mathbb{R}^n, B_0 \in \mathbb{R}^{n \times n}.$$

Get $Q_0 \mathbb{R}_0 = B_0$
 $L_0 \text{ from } \mathbb{R}^\top$
 $D_0 = (r_{11}^2, \dots, r_{nn}^2).$

Do for
$$k = 1, ...$$
:
Solve $L_k D_k L_k^\top s_k = -B_k^\top f(x_k)$ for s_k ,
 $x_{k+1} := x_k + s_k$,
 $y_k := f(x_{k+1}) - f(x_k)$,
 $t_k := -B_k^\top f(x_k)$.
 $B_{k+1} := B_k + \frac{(y_k - B_k s_k) s_k^\top}{s_k^\top s_k}$.
Get $\tilde{L} \tilde{D} \tilde{L}^\top$, \overline{LDL}^\top by Algorithm 2.1

In the next section, we will give a convergence analysis of Algorithm 2.2.

A Method Using the Convex Update

We will first describe the Quasi-Gauss-Newton method using the convex update:

$$\Delta B = (1 - \mu)\Delta B_1 + \mu \Delta B_2,$$

where $\mu = \frac{(s^{\top}t)^2}{(s^+s)(t^+t)}$. Therefore,

$$\overline{B} = B + \Delta B$$

= $B + (1 - \mu)\Delta B_1 + \mu\Delta B_2$
= $B + \overline{f}z^{\top}$, (10)

where $z = (1 - \mu)\frac{s}{s^{\top}s} + \mu \frac{t}{t^{\top}s}$. If (10) is used for the Jacobian approximation in (8), then we are led to an updating scheme to get $\overline{B}^{\top}\overline{B}$ from $B^{\top}B$ as follows.

LEMMA 2.3. Let $\tau = \overline{f}^{\top} \overline{f}$ and $\overline{t} = -\overline{B}^{\top} \overline{f}$, then,

$$\overline{B}^{\mathsf{T}}\overline{B} = B^{\mathsf{T}}B - \overline{t}z^{\mathsf{T}} - z^{\mathsf{T}}\overline{t}^{\mathsf{T}} - \tau z z^{\mathsf{T}}.$$
(11)

If we let

$$z_1 = \frac{-\bar{t} + (1 - \tau/2)z}{\sqrt{2}}$$
 and $z_2 = \frac{-\bar{t} - (1 + \tau/2)z}{\sqrt{2}}$

then

$$\overline{B}^{\mathsf{T}}\overline{B} = B^{\mathsf{T}}B + z_1 z_1^{\mathsf{T}} - z_2 z_2^{\mathsf{T}}.$$

Proof.

$$\overline{B}^{\top}\overline{B} = (B + \Delta B)^{\top}(B + \Delta B)$$
$$= B^{\top}B + \Delta B^{\top}B + B^{\top}\Delta B + \Delta B^{\top}\Delta B.$$

Since $B = (\overline{B} - \Delta B)$,

$$B^{\top} \Delta B = \left(\overline{B} - \Delta B\right)^{\top} \Delta B$$
$$= \overline{B}^{\top} \overline{f} z^{\top} - \Delta B^{\top} \Delta B$$
$$= -\overline{t} z^{\top} - \tau z z^{\top}.$$

Similarly, $\Delta B^{\mathsf{T}}B = -z\overline{t}^{\mathsf{T}} - \tau z z^{\mathsf{T}}$. From $\Delta B^{\mathsf{T}}\Delta B = \tau z z^{\mathsf{T}}$ and the above equations, (11) follows. In view of

$$z_{1}z_{1}^{\top} = \frac{1}{2} \left[-\overline{t} + \left(\frac{1-\tau}{2}\right)z \right] \left[-\overline{t}^{\top} + \left(\frac{1-\tau}{2}\right)z^{\top} \right]$$
$$= \frac{1}{2} \left[\overline{t}\overline{t}^{\top} - \left(\frac{1-\tau}{2}\right)\overline{t}z^{\top} - \left(\frac{1-\tau}{2}\right)z\overline{t}^{\top} + \left(\frac{1-\tau}{2}\right)^{2}zz^{\top} \right]$$

and

$$z_2 z_2^{\mathsf{T}} = \frac{1}{2} \left[\overline{t} \overline{t}^{\mathsf{T}} + \left(\frac{1-\tau}{2} \right) \overline{t} z^{\mathsf{T}} + \left(\frac{1-\tau}{2} \right) z \overline{t}^{\mathsf{T}} + \left(\frac{1-\tau}{2} \right)^2 z z^{\mathsf{T}} \right],$$

we have

$$z_1 z_1^{\top} - z_2 z_2^{\top} = -\overline{t} z^{\top} - z^{\top} \overline{t}^{\top} - \tau z z^{\top}.$$

Since the equation,

$$B^{\mathsf{T}}Bs = -B^{\mathsf{T}}f$$

must be solved for s and this involves $O(n^3)$ operations per iteration, we apply the techniques in Algorithm 2.2 for implementing this method. The initial L and D are obtained from

$$B^{\top}B = R^{\top}Q^{\top}QR = R^{\top}R,$$

by letting $R^{\top}R = LDL^{\top}$. This implies that

$$D_{i,i} = \left(r_{ii}^2\right),\,$$

then L is obtained from R^{\top} by dividing the i^{th} row of R^{\top} by the i^{th} diagonal element of R, $i = 1, \ldots, n$.

Algorithm 2.1 is for rank-1 update and $B^{\top}B$ is rank-2, as shown in Lemma 2.3, hence, Algorithm 2.1 will be applied twice. The algorithm for the proposed method is as follows.

Algorithm 2.4.

Given
$$f: \mathbb{R}^n \to \mathbb{R}^n, x_0 \in \mathbb{R}^n, B_0 \in \mathbb{R}^{n \times n}.$$

Get $Q_0 \mathbb{R}_0 = \mathbb{B}_0$
 $L_0 \text{ from } \mathbb{R}^\top$
 $D_0 = (r_{11}^2, \dots, r_{nn}^2).$

Do for
$$k = 1, \dots$$
:
Solve $L_k D_k L_k^{\top} s_k = -B_k^{\top} f(x_k)$ for s_k ,
 $x_{k+1} := x_k + s_k$,
 $y_k := f(x_{k+1}) - f(x_k)$,
 $t_k := -B_k^{\top} f(x_k)$.
 $B_{k+1} := B_k + (1-\mu) \frac{(y_k - B_k s_k) s_k^{\top}}{s_k^{\top} s_k} + \mu \frac{(y_k - B_k s_k) t_k^{\top}}{t_k^{\top} s_k}$.
Get $\tilde{L} \tilde{D} \tilde{L}^{\top}, \overline{LDL^{\top}}$ by Algorithm 2.1.

3. CONVERGENCE ANALYSIS

In this section, we prove that the methods defined by (9) and (11) are well defined and converge to a solution of (1). We also give a comparison of the convergence rates of two methods.

Convergence of QGN Method

THEOREM 3.1. (THE BOUNDED DETERIORATION THEOREM). Let $D \subseteq \mathbb{R}^n$ be an open convex set containing x, \overline{x} , with $x \neq x^*$. Let $f : \mathbb{R}^n \to \mathbb{R}^n$, $B \in \mathbb{R}^{n \times n}$, $\overline{B}^\top \overline{B}$ defined by (9). If $x^* \in D$ and J(x) obeys the weaker Lipschitz condition,

$$\left\|J(x) - J(x^*)\right\| \le \gamma \left\|x - x^*\right\|, \qquad \text{for all } x \in D,$$

then, for both the Frobenius and l_2 matrix norms,

$$\left\| \left(\overline{B} - J(x^*) \right)^\top \left(\overline{B} - J(x^*) \right) \right\| \le \left[\|B - J(x^*)\| + \frac{\gamma}{2} \left(\|\overline{x} - x^*\|_2 + \|x - x^*\|_2 \right) \right]^2.$$
(12)

PROOF. Let $J_* \equiv J(x^*)$. Adding $-J_*^\top \overline{B} - \overline{B}^\top J + J_*^\top J_*$ to the both sides of (9), we get

$$\overline{B}^{\mathsf{T}}\overline{B} - J_{\star}^{\mathsf{T}}\overline{B} - \overline{B}^{\mathsf{T}}J + J_{\star}^{\mathsf{T}}J_{\star} = B^{\mathsf{T}}B - J_{\star}^{\mathsf{T}}\overline{B} - \overline{B}^{\mathsf{T}}J + J_{\star}^{\mathsf{T}}J_{\star} + B^{\mathsf{T}}\frac{(y - Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \frac{s(y - Bs)^{\mathsf{T}}}{s^{\mathsf{T}}s}B + \frac{s(y - Bs)^{\mathsf{T}}}{s^{\mathsf{T}}s}\frac{(y - Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} = \left[B - J_{\star} + \frac{(y - Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right]^{\mathsf{T}} \left[B - J_{\star} + \frac{(y - Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right] = \left[(B - J_{\star})\left[I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right] + \frac{(y - J_{\star}s)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right]^{\mathsf{T}} \times \left[(B - J_{\star})\left[I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right] + \frac{(y - J_{\star}s)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right].$$
(13)

Then, it follows that

$$\left\| \left(\overline{B} - J_{*}\right)^{\mathsf{T}} \left(\overline{B} - J_{*}\right) \right\| \leq \left[\left\| \left(B - J_{*}\right) \left[I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right] \right\| + \frac{\|y - J_{*}s\|_{2}}{\|s\|_{2}} \right]^{2}$$

Using

$$\left\|I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right\|_2 = 1,$$

and

$$\|y - J_*s\|_2 \le \frac{\gamma}{2} \left(\|\overline{x} - x_*\|_2 + \|x - x_*\|_2\right) \|s\|_2$$

in [6], we have (12).

The linear convergence of the Quasi-Gauss-Newton method can be proved by using Theorem 3.1 and induction to show that $||(B_k - J_*)^{\top}(B_k - J_*)|| \leq [(2 - 2^{-k})\delta]^2$ and $||e_{k+1}|| \leq (||e_k||/2)$, for $k = 0, 1, 2, \ldots$, where $||B_0 - J_*|| < \delta$.

We will now prove the superlinear convergence of the method by showing that

$$\lim_{n \to \infty} \frac{\left\| (B_k - J(x^*))^\top (B_k - J(x^*)) s_k \right\|}{\|s\|} = 0.$$
(14)

We need the following lemma for the proof.

LEMMA 3.2. Let $s \in \mathbb{R}^n$ be nonzero, $E \in \mathbb{R}^{n \times n}$, and let $\|\cdot\|$ denote the l_2 vector norm, then,

$$\begin{split} \left\| \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right)^{\mathsf{T}} E^{\mathsf{T}} E \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right) \right\|_{F} &= \left(\left\| E^{\mathsf{T}} E \right\|_{F}^{2} - \left\| E^{\mathsf{T}} E \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right\|_{F}^{2} \right)^{(1/2)} \\ &\leq \left\| E^{\mathsf{T}} E \right\|_{F} - \frac{1}{2 \left\| E^{\mathsf{T}} E \right\|_{F}} \left(\frac{\left\| E^{\mathsf{T}} E s \right\|^{2}}{\left\| s \right\|^{2}} \right). \end{split}$$

PROOF. We have

$$\left\| \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right)^{\mathsf{T}} E^{\mathsf{T}} E \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right) \right\|_{F} = \left\| E \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right) \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right) E^{\mathsf{T}} \right\|_{F} = \left\| E \left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right) E^{\mathsf{T}} \right\|_{F}$$

and

$$\left\|E^{\mathsf{T}}E\right\|_{F}^{2} = \left\|E^{\mathsf{T}}E\left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right)\right\|_{F}^{2} + \left\|E^{\mathsf{T}}E\frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right\|_{F}^{2},$$

therefore,

$$\begin{split} \left\| E^{\mathsf{T}} E\left(I - \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right) \right\|_{F} &= \left(\left\| E^{\mathsf{T}} E \right\|_{F}^{2} - \left\| E^{\mathsf{T}} E \frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s} \right\|_{F}^{2} \right)^{(1/2)} \\ &\leq \left\| E^{\mathsf{T}} E \right\|_{F} - \frac{1}{2 \left\| E^{\mathsf{T}} E \right\|_{F}} \left(\frac{\left\| E^{\mathsf{T}} Es \right\|^{2}}{\left\| s \right\|^{2}} \right), \end{split}$$

since $||E^{\top}E||_F \ge ||E^{\top}E\frac{ss^{\top}}{s^{\top}s}||_F \ge 0.$

THEOREM 3.3. (SUPERLINEAR CONVERGENCE). Let all the assumptions of Theorem 3.1 hold. Then, the sequence $\{x_k\}$ generated by Algorithm 2.2 is well defined and converges superlinearly to x^* .

PROOF. Define $E_k = B_k - J_*$, and let $\|\cdot\|$ denote the l_2 vector norm. From (13),

$$\begin{split} \left\| E_{k+1}^{\top} E_{k+1} \right\|_{F} &\leq \left\| \left(I - \frac{s_{k} s_{k}^{\top}}{s_{k}^{\top} s_{k}} \right) E_{k}^{\top} E_{k} \left(I - \frac{s_{k} s_{k}^{\top}}{s_{k}^{\top} s_{k}} \right) \right\|_{F} + 2 \left\| E_{k} \left(I - \frac{s_{k} s_{k}^{\top}}{s_{k}^{\top} s_{k}} \right) \right\|_{F} \frac{\| y_{k} - J_{*} s_{k} \|_{2}}{\| s_{k} \|_{2}} \\ &+ \left(\frac{\| y_{k} - J_{*} s_{k} \|_{2}}{\| s_{k} \|_{2}} \right)^{2}. \end{split}$$

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Using $\frac{\|y - J_{\bullet} s_k\|_2}{\|s_k\|_2} \le (\gamma/2)(\|e_k\|_2 + \|e_{k+1}\|_2)$, Lemma 3.2, and $\|e_{k+1}\| \le (1/2)\|e_k\|$,

$$\left\|E_{k+1}^{\top}E_{k+1}\right\|_{F} \leq \left\|E_{k}^{\top}E_{k}\right\|_{F} - \frac{1}{2\left\|E_{k}^{\top}E_{k}\right\|_{F}} \frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} + \frac{3\gamma\left\|E_{k}\right\|_{F}}{2}\left\|e_{k}\right\| + \frac{9\gamma}{16}\left\|e_{k}\right\|^{2}.$$

This can be rewritten as

$$\frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} \leq 2\left\|E_{k}^{\top}E_{k}\right\|_{F}\left[\left\|E_{k}^{\top}E_{k}\right\|_{F} - \left\|E_{k+1}^{\top}E_{k+1}\right\|_{F} + \frac{3\gamma}{2}\left\|E_{k}\right\|\left\|e_{k}\right\| + \frac{9\gamma}{16}\left\|e_{k}\right\|^{2}\right].$$

From the proof of the linear convergence, $||E_k^{\top}E_k||_F \leq 4\delta^2$ and $||E_k|| \leq 2\delta$ for all $k \geq 0$, $\sum_{k=0}^{\infty} ||e_k|| \leq 2\epsilon$, and $\sum_{k=0}^{\infty} ||e_k||^2 \leq (4/3)\epsilon$,

$$\frac{\left|E_{k}^{\top}E_{k}s_{k}\right|^{2}}{\left\|s_{k}\right\|^{2}} \leq 4\delta^{2}\left[\left\|E_{k}^{\top}E_{k}\right\|_{F} - \left\|E_{k+1}^{\top}E_{k+1}\right\|_{F} + 3\delta\gamma\left\|e_{k}\right\| + \frac{9\gamma}{16}\left\|e_{k}\right\|^{2}\right].$$

Summing for $k = 0, 1, \ldots, i$,

$$\begin{split} \sum_{k=0}^{i} \frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} &\leq 4\delta^{2} \left[\left\|E_{0}^{\top}E_{0}\right\|_{F} - \left\|E_{i+1}^{\top}E_{i+1}\right\|_{F} + 3\delta\gamma\sum_{k=0}^{i}\left\|e_{k}\right\| + \frac{9\gamma}{16}\sum_{k=0}^{i}\left\|e_{k}\right\|^{2}\right] \\ &\leq 4\delta^{2} \left[\left\|E_{0}^{\top}E_{0}\right\|_{F} + 6\delta\gamma\epsilon + \frac{3}{4}\gamma\epsilon\right] \\ &\leq 4\delta^{2} \left[4\delta^{2} + 6\delta\gamma\epsilon + \frac{3}{4}\gamma\epsilon\right], \end{split}$$

which shows that

$$\sum_{k=0}^{i} \frac{\left\| E_{k}^{\top} E_{k} s_{k} \right\|^{2}}{\left\| s_{k} \right\|^{2}}$$

is finite. This implies (14). Therefore, the Quasi-Gauss-Newton method converges superlinearly.

Convergence of the Proposed Method

Next, we show the convergence of the method defined by (11) by starting with the bounded deterioration theorem.

THEOREM 3.4. (THE BOUNDED DETERIORATION THEOREM). Let all the assumptions of Theorem 3.1 hold and $B \in \mathbb{R}^{n \times n}$, $\overline{B}^{\top}\overline{B}$ defined by (11). If $x^* \in D$ and J(x) obeys the weaker Lipschitz condition, then, for both the Frobenius and l_2 matrix norms,

$$\left\| \left(\overline{B} - J(x^*) \right)^{\top} \left(\overline{B} - J(x^*) \right) \right\|_{F} \le \left[\|B - J(x^*)\|_{F} + \frac{\gamma}{2} \left(\|\overline{x} - x^*\|_{2} + \|x - x^*\|_{2} \right) \right]^{2}.$$
(15)

PROOF. Let $J_* \equiv J(x^*)$. Adding $-J_*^\top \overline{B} - \overline{B}^\top J + J_*^\top J_*$ to the both sides of (11),

$$\overline{B}^{\mathsf{T}}\overline{B} - J_{*}^{\mathsf{T}}\overline{B} - \overline{B}^{\mathsf{T}}J + J_{*}^{\mathsf{T}}J_{*} = B^{\mathsf{T}}B - J_{*}^{\mathsf{T}}\overline{B} - \overline{B}^{\mathsf{T}}J + J_{*}^{\mathsf{T}}J_{*}
+ B^{\mathsf{T}}\left[(1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right] + \left[(1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right]^{\mathsf{T}}B
+ \left[(1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right]^{\mathsf{T}}\left[(1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right]
= \left[B - J_{*} + (1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right]^{\mathsf{T}}\left[B - J_{*}(1-\mu)\frac{(y-Bs)s^{\mathsf{T}}}{s^{\mathsf{T}}s} + \mu\frac{(y-Bs)t^{\mathsf{T}}}{t^{\mathsf{T}}s}\right]
= \left[(B - J_{*})\left[I - P\right] + \frac{(y - J_{*}s)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right]^{\mathsf{T}}\left[(B - J_{*})\left[I - P\right] + \frac{(y - J_{*}s)s^{\mathsf{T}}}{s^{\mathsf{T}}s}\right],$$
(16)

where $P = \frac{ss^{\top}}{s^{\top}s} \left[(1-\mu)I + \frac{tt^{\top}}{t^{\top}t} \right]$. Then,

$$\left\| \left(\overline{B} - J_* \right)^{\mathsf{T}} \left(\overline{B} - J_* \right) \right\|_F \le \left[\left\| (B - J_*) \left(I - P \right) \right\|_F + \frac{\|y - J_* s\|_2}{\|s\|_2} \right]^2.$$

Using

$$||I - P||_2 = 1,$$

 and

$$||y - J_*s||_2 \le \frac{\gamma}{2} (||\overline{x} - x^*||_2 + ||x - x^*||_2) ||s||_2$$

we have (15).

We need the following lemmas to prove the convergence of the method defined by (11).

LEMMA 3.5. If $P = \frac{ss^{\top}}{s^{\top}s} \left[(1-\mu)I + \frac{tt^{\top}}{t^{\top}t} \right]$, where $t = -B^{\top}f$ and $\mu = \frac{(s^{\top}t)^2}{s^{\top}st^{\top}t}$, then $(I-P)(I-P)^{\top}$ is a projector.

PROOF. We first show that $[(I-P)(I-P)^{\top}]^2 = (I-P)(I-P)^{\top}$. Using $PP^{\top} = (1-\mu^2+\mu)\frac{ss^{\top}}{s^{\top}s}$,

$$(I - P) (I + PP^{\top}) = (I - P) \left(I + (1 - \mu^{2} + \mu) \frac{ss^{\top}}{s^{\top}s} \right)$$

= $I - P + (1 - \mu^{2} + \mu) \frac{ss^{\top}}{s^{\top}s} - (1 - \mu^{2} + \mu) \left[(1 - \mu) \frac{ss^{\top}}{s^{\top}s} + \mu \frac{st^{\top}}{t^{\top}s} \right] \frac{ss^{\top}}{s^{\top}s}$
= $I - P + (1 - \mu^{2} + \mu) \frac{ss^{\top}}{s^{\top}s} - (1 - \mu^{2} + \mu) \left[(1 - \mu) \frac{ss^{\top}}{s^{\top}s} + \mu \frac{ss^{\top}}{s^{\top}s} \right]$
= $I - P$.

Hence,

$$(I - P)(I - P)^{\mathsf{T}}(I - P)(I - P)^{\mathsf{T}} = (I - P)(I - P)^{\mathsf{T}} + P^{\mathsf{T}}P(I - P)^{\mathsf{T}} - PP^{\mathsf{T}}P(I - P)^{\mathsf{T}}$$

= $(I - P)(I - P)^{\mathsf{T}} + (I - P)P^{\mathsf{T}}P(I - P)^{\mathsf{T}}$
= $(I - P)(I + P^{\mathsf{T}}P)(I - P)^{\mathsf{T}}$
= $(I - P)(I - P)^{\mathsf{T}}$.

Therefore, $(I - P)(I - P)^{\top}$ is a projector.

LEMMA 3.6. If P is given as Lemma 3.5, then

$$\left\| (I-P)^{\top} E^{\top} E(I-P) \right\|_{F} = \left\| E^{\top} E(I-P) \right\|_{F} \le \left\| E^{\top} E \right\|_{F} - \frac{1-\mu^{2}+\mu}{2 \left\| E^{\top} E \right\|_{F}} \frac{\left\| E^{\top} E s \right\|^{2}}{\|s\|^{2}}.$$

PROOF. Using Lemma 3.5,

$$\begin{aligned} \left\| (I-P)^{\top} E^{\top} E(I-P) \right\|_{F}^{2} &= \left\| E^{\top} E(I-P)(I-P)^{\top} \right\|_{F}^{2} \\ &= \operatorname{tr} \left(E^{\top} E(I-P)(I-P)^{\top} (I-P)(I-P)^{\top} E^{\top} E \right) \\ &= \operatorname{tr} \left(E^{\top} E(I-P)(I-P)^{\top} E^{\top} E \right) \\ &= \left\| E^{\top} E(I-P) \right\|_{F}^{2}. \end{aligned}$$

Since $P^2 = P$, we have

$$\begin{split} \left\| E^{\top} E(I-P) \right\|_{F}^{2} &= \left\| E^{\top} E \right\|_{F}^{2} - \left\| E^{\top} E P \right\|_{F}^{2} .\\ \left\| E^{\top} E(I-P) \right\|_{F} &\leq \left\| E^{\top} E \right\|_{F} - \frac{1}{2 \left\| E^{\top} E \right\|_{F}} \left\| E^{\top} E P \right\|_{F}^{2} \\ &= \left\| E^{\top} E \right\|_{F} - \frac{1 - \mu^{2} + \mu}{2 \left\| E^{\top} E \right\|_{F}} \frac{\left\| E^{\top} E s \right\|_{F}^{2}}{\left\| s \right\|^{2}} \end{split}$$

from $||E^{\top}E||_F \ge ||E^{\top}EP||_F$.

The convergence theorem is given as follows.

THEOREM 3.7. Let all the assumptions of Theorem 3.1 hold. Let $E = B_k - J_*$. Then, $\{x_k\}$ generated by Algorithm 2.4 converges superlinearly.

PROOF. From (16),

$$\begin{split} \left\| E_{k+1}^{\mathsf{T}} E_{k+1} \right\|_{F} &\leq \left\| (I-P)^{\mathsf{T}} E_{k}^{\mathsf{T}} E_{k} (I-P) \right\|_{F} + 2 \left\| E_{k} (I-P) \right\|_{F} \frac{\left\| (y_{k} - J_{*} s_{k}) \right\|_{2}}{\left\| s_{k} \right\|_{2}} \\ &+ \left(\frac{\left\| (y_{k} - J_{*} s_{k}) \right\|_{2}}{\left\| s_{k} \right\|_{2}} \right)^{2}. \end{split}$$

By $\frac{\|(y_k - J_* s_k)\|_2}{\|s_k\|_2} \le (\gamma/2)(\|e_k\|_2 + \|e_{k+1}\|_2)$ and $\|e_{k+1}\| \le \frac{\|e_k\|}{2}$, we have

$$\begin{split} \left\| E_{k+1}^{\top} E_{k+1} \right\|_{F} &\leq \left\| (I-P)^{\top} E_{k}^{\top} E_{k} (I-P) \right\|_{F} + \frac{3\gamma}{2} \left\| E_{k} (I-P) \right\|_{F} \left\| e_{k} \right\| + \frac{9\gamma}{16} \left\| e_{k} \right\|^{2} \\ &= \left\| E_{k}^{\top} E_{k} (I-P) \right\|_{F} + \frac{3\gamma}{2} \left\| E_{k} (I-P) \right\|_{F} \left\| e_{k} \right\| + \frac{9\gamma}{16} \left\| e_{k} \right\|^{2}. \end{split}$$

From Lemma 3.6,

$$\left\|E_{k+1}^{\top}E_{k+1}\right\|_{F} \leq \left\|E_{k}^{\top}E_{k}\right\|_{F} - \frac{1-\mu^{2}+\mu}{2\left\|E_{k}^{\top}E_{k}\right\|_{F}} \frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} + \frac{3\gamma}{2}\left\|E_{k}\right\|_{F}\left\|e_{k}\right\| + \frac{9\gamma}{16}\left\|e_{k}\right\|^{2}.$$

This can be rewritten as

$$\frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} \leq \frac{2\left\|E_{k}^{\top}E_{k}\right\|_{F}}{\left(1-\mu^{2}+\mu\right)} \left[\left\|E_{k}^{\top}E_{k}\right\|_{F}-\left\|E_{k+1}^{\top}E_{k+1}\right\|_{F}+\frac{3\gamma}{2}\left\|E_{k}\right\|_{F}\left\|e_{k}\right\|+\frac{9\gamma}{16}\left\|e_{k}\right\|^{2}\right].$$

Since $||E_k||_F \leq 2\delta$ for all $k \geq 0$, $\sum_{k=0}^{\infty} ||e_k|| \leq 2\epsilon$, and $\sum_{k=0}^{\infty} ||e_k||^2 \leq (4/3)\epsilon$,

$$\frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} \leq \frac{4\delta^{2}}{(1-\mu^{2}+\mu)} \left[\left\|E_{k}^{\top}E_{k}\right\|_{F} - \left\|E_{k+1}^{\top}E_{k+1}\right\|_{F} + 3\gamma\delta\left\|e_{k}\right\| + \frac{9\gamma}{16}\left\|e_{k}\right\|^{2}\right].$$

Summing for $k = 0, 1, \ldots, i$,

$$\sum_{k=0}^{i} \frac{\left\|E_{k}^{\top}E_{k}s_{k}\right\|^{2}}{\left\|s_{k}\right\|^{2}} \leq \frac{4\delta^{2}}{(1-\mu^{2}+\mu)} \left[\left\|E_{0}^{\top}E_{0}\right\|_{F} - \left\|E_{i+1}^{\top}E_{i+1}\right\|_{F} + 3\gamma\delta\sum_{k=0}^{i}\left\|e_{k}\right\| + \frac{9\gamma}{16}\sum_{k=0}^{i}\left\|e_{k}\right\|^{2}\right] \\ \leq \frac{4\delta^{2}}{(1-\mu^{2}+\mu)} \left[\left\|E_{0}^{\top}E_{0}\right\|_{F} + 6\delta\gamma\epsilon + \frac{3\gamma}{4}\epsilon\right] \\ \leq \frac{4\delta^{2}}{(1-\mu^{2}+\mu)} \left[\delta^{2} + 6\delta\gamma\epsilon + \frac{3\gamma}{4}\epsilon\right].$$
(17)

Equation (17) holds for all i,

$$\sum_{k=0}^{i} \left[\frac{\left\| E_k^{\top} E_k s_k \right\|^2}{\left\| s_k \right\|^2} \right]$$

is finite. This implies (14). Therefore, Algorithm 2.4 converges superlinearly. Since $(1-\mu^2+\mu) \leq 1$, the bound for the new algorithm is smaller than that of Theorem 3.4.

Comparison of the Convergence Rates

We show that the new algorithm's approximation to $F'(x_k)$ at each iteration is better than that of Broyden's. In the next lemma, we compare the bounds of the bounded deterioration theorems of the both methods.

THEOREM 3.8. If B_k and \overline{B}_k are, respectively, approximations for the Jacobians of the methods defined by (9) and (11), then,

$$\left\| \left(\overline{B}_k - J_* \right)^\top \left(\overline{B}_k - J_* \right) \right\|_F \le \left\| \left(B_k - J_* \right)^\top \left(B_k - J_* \right) \right\|_F$$

PROOF. Let $E_k = B_k - J_*$ and $\overline{E}_k = \overline{B}_k - J_*$, then, from Theorem 3.1, we have

$$\left\|E_{k}^{\mathsf{T}}E_{k}\right\|_{F} \leq \left[\left\|E_{k-1}^{\mathsf{T}}E_{k-1}\left(I-\frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right)\right\|_{F}+\frac{\left\|(y_{k-1}-J_{*}s)\right\|_{2}}{\|s\|_{2}}\right]^{2},$$

and for the method of (11) from Theorem 3.4,

$$\left\|\overline{E}_{k}^{\top}\overline{E}_{k}\right\|_{F} \leq \left[\left\|E_{k-1}^{\top}E_{k-1}(I-P)\right\|_{F} + \frac{\left\|(y_{k-1}-J_{*}s)\right\|_{2}}{\|s\|_{2}}\right]^{2}.$$

From Lemmas 3.2 and 3.6,

$$\|E^{\top}E(I-P)\|_{F}^{2} = \|E^{\top}E\|_{F}^{2} - (1-\mu^{2}+\mu)\left(\frac{\|E^{\top}Es\|}{\|s\|}\right)^{2},$$

and

$$\left\|E^{\mathsf{T}}E\left(I-\frac{ss^{\mathsf{T}}}{s^{\mathsf{T}}s}\right)\right\|_{F}^{2}=\left\|E^{\mathsf{T}}E\right\|^{2}-\left(\frac{\left\|E^{\mathsf{T}}Es\right\|}{\left\|s\right\|}\right)^{2}.$$

Since $\mu \leq 1$ and $1 - \mu^2 + \mu \geq 1$, we have

$$\|E^{\mathsf{T}}E\|_{F}^{2} - (1 - \mu^{2} + \mu)\left(\frac{\|E^{\mathsf{T}}Es\|}{\|s\|}\right)^{2} \le \|E^{\mathsf{T}}E\|_{F}^{2} - \left(\frac{\|E^{\mathsf{T}}Es\|}{\|s\|}\right)^{2},$$

which proves $||E^{\top}E(I-P)||_F \leq ||E^{\top}E\left(I-\frac{ss^{\top}}{s^{\top}s}\right)||_F$. Therefore, we get $||\overline{E}_k^{\top}\overline{E}_k||_F \leq ||E_k^{\top}E_k||_F$.

Computational Results

Results of computational experiments are summarized in Table 1. The computations were done on a Sun Sparc II. All the nonlinear nonsymmetric problems in the set of test problems [7,8] were utilized. The problems are numbered as in [7] and Problem 31 was modified as in [1]. Initial Jacobians were evaluated numerically by finite differences. In Table 1, the performance of the proposed method is compared with Quasi-Gauss-Newton method when n = 100. It is clear from Table 1, that the proposed method shows better performance than Quasi-Gauss-Newton method. This agrees with the proof in the previous section. It may appear that the number of operations for the proposed method is larger than that of Quasi-Gauss-Newton method, since it combines the two updates for the Jacobian approximation, however, Quasi-Gauss-Newton method also includes the operations to compute $t = -B^{\top} f$ according to (3). Hence, the number of operations for the two methods is almost same. For all problems tested, the proposed method has the same or better rate of convergence and run time than Quasi-Gauss-Newton method. For Problem 31, the proposed method performs better than Quasi-Gauss-Newton method as the scaling gets worse.

| Problem | Quasi-Gauss-Newton Method | | Proposed Method | |
|---------|---------------------------|-----------------|-------------------|-----------------|
| Number | No. of Iterations | Time in Seconds | No. of Iterations | Time in Seconds |
| 21 | Diverged | - | Diverged | - |
| 22 | 19 | 4.900 | 19 | 4.900 |
| 26 | 83 | 20.740 | 82 | 20.630 |
| 27 | Diverged | - | Diverged | _ |
| 28 | 2 | 2.390 | 2 | 2.390 |
| 29 | 4 | 2.810 | 4 | 2.810 |
| 30 | 8 | 3.230 | 8 | 3.230 |
| 31(1) | 14 | 5.840 | 14 | 5.830 |
| 32(2) | 18 | 6.500 | 18 | 6.490 |
| 31(3) | 28 | 8.110 | 18 | 6.510 |
| 31(4) | 30 | 8.440 | 22 | 7.140 |
| 31(5) | 6 | 9.420 | 30 | 8.450 |
| 31(6) | 55 | 12.520 | 37 | 9.600 |
| 31(7) | 139 | 26.280 | 44 | 10.870 |

Table 1. Proposed Method vs. Quasi-Gauss-Newton Method.

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