Comm. Korean Math. Soc. 9 (1994), No. 3, pp. 739–751

ON IMPROVING GAUSS-NEWTON METHOD FOR NONLINEAR EQUATIONS

SUNYOUNG KIM

1. Introduction

We consider the following problem.

Determine a point $x^* = (x_1^*, \dots, x_n^*)^T$
for given function $f_k(x) = f_k(x_1, \dots, x_n),\ k = 1, \dots, n$

$$f(x) = \begin{bmatrix} f_1(x_1, \dots, x_n) \\ \cdot \\ \cdot \\ \cdot \\ f_n(x_1, \dots, x_n) \end{bmatrix}$$

which satisfies

$$f(x^*) = 0. \tag{1}$$

The classical methods to (1) are Newton's method, Broyden method [1] in Quasi-Newton class ([2], [7], [9], [10]), Gauss-Newton method [8] which approximates $f_k, k = 1, .., n$ by a linear function. A linearization technique is: If we assume that $x = \xi$ is a zero for f, that x_0 is an approximation to ξ, and that f is differentiable for $x = x_0$, then to a first approximation

$$0 = f(\xi) \approx f(x_0) + Df(x_0)(\xi - x_0),$$

where $Df(x_0)$ is the Jacobian at x_0. If the Jacobian $Df(x_0)$ is nonsingular, then the equation

$$f(x_0) + Df(x_0)(x_1 - x_0) = 0 \tag{2}$$

Received January 19, 1994.
This work was supported by the Ministry of Education.

can be solved for x_1:

$$x_1 = x_0 - (Df(x_0))^{-1} f(x_0)$$

and x_1 may be taken as a closer approximation to the zero ξ. The differences between Newton's method and Gauss-Newton method lie on how the Jacobian is obtained and the equation (3).

The generalized Newton method for solving systems of equations is given for

$$x_{i+1} = x_i - (Df(x_i))^{-1} f(x_i), \; i = 0, 1, 2, \ldots \tag{3}$$

If we let $x_i = x$ and $x_{i+1} = \overline{x}$, then

$$f(\overline{x}) = f(x) + Df(x)(\overline{x} - x) + h, \; \| h \| = o(\| \overline{x} - x \|).$$

If x is close to the solution of (1), then the solution $\overline{x}$ of

$$min_{z \in R^n} \| f(x) + Df(x)(z - x) \|^2 = \| f(x) + Df(x)(\overline{x} - x) \|^2,$$

will be still closer than x;

$$\| f(\overline{x}) \|^2 < \| f(x) \|^2 .$$

This is not always true in the form given. However, if the direction is defined as

$$s = s(x) := \overline{x} - x$$

then, there is a $\lambda > 0$ such that the function,

$$\phi(\tau) := \| f(x + \tau s) \|^2,$$

is strictly monotone decreasing for all $0 \leq \tau \leq \lambda$ [14]. In particular,

$$\phi(\lambda) = \| f(x + \lambda s) \|^2 < \phi(0) = \| f(x) \|^2 .$$

Newton's method described above is the most fundamental but has computational difficulty in practical environment [4]. In Gauss-Newton method, the next iterate x_{i+1} is obtained by solving the normal equation,

$$Df(x_i)^T Df(x_i) s = -Df(x_i)^T f(x_i).$$

Gauss-Newton method is known to be among the best available technique for nonlinear problems in practice. However, it shows lack of reliability. That is, Gauss-Newton method either performs very well, or else it performs very poorly on a particular problem compared to other methods. Therefore, it is very hard to predict the behavior of Gauss-Newton method when considering large and varied sets of test problems. It is also known that Gauss-Newton method is not a good approach for the problems with nearly rank deficient Jacobians. There are many cases that Gauss-Newton method fail or are inefficient [8]. In this paper, we are mainly concerned with improving Gauss-Newton method with a new Jacobian estimate. To accomplish this, we use an update proposed in the next section as Jacobian estimate in Gauss-Newton method and compare its computational performance with Gauss-Newton method using Broyden's update on the given set of test problems. In section 2, we describe Broyden update and a weighted update and measure how close they can estimate the Jacobian. In section 3, Gauss-Newton methods employing the updates in section 2 are given. We also present a new Gauss-Newton algorithm which modifies the Gauss-Newton coefficient matrix by the weighted method. In section 4, numerical results for the methods in section 2 and 3 are shown. Throughout this paper, we use the Frobenius norm defined as $\| A \|_F^2 = tr(AA^T)$ and the weighted Frobenius norm $\| A \|_{M,F} = \| AMA^T \|_F$.

2. Updates

In this section, we describe Broyden's update and propose a weighted update and a combination of the two updates. We also present Theorems to measure the updates' closeness to the Jacobian.

If B_i and B_{i+1} are Jacobian estimates for i-th and $i+1$-th iteration, respectively, and $B_{i+1} = B_i + \Delta B$, then ΔB is called an update. The update used in Broyden's method is called Broyden's update. The normal equation in Gauss-Newton method involves the Jacobian, which is usually replaced by Broyden's update for computational efficiency.

Broyden's update (M1)

The Broyden update, say ΔB_1, is

$$\Delta B_1 = \sigma \overline{f} s^T, \tag{4}$$

where $\sigma = (s^Ts)^{-1}$ as in [2]. ΔB_1 minimizes $\| \Delta B \| = \text{Trace}(\Delta B \Delta B^T)$, viz., the sum of the squares of the elements of ΔB [15]. Namely, ΔB_1 is the least change update in $\| \cdot \|_F$.

A Weighted Method (M2)

On the other hand, it is shown that in [15] that the update,

$$\Delta B_2 = \overline{f} \frac{s^T V}{s^T V s}, \tag{5}$$

minimizes

$$\| \Delta B \|_{V^{-1}} = \text{Trace}(\Delta B V^{-1} \Delta B^T). \tag{6}$$

V can be any choice of matrices. If we choose $V = B^T B$ and let $t = -B^T f$, then, using $Bs = -f$ from (3), we have $Vs = B^T Bs = -B^T f = t$ and (5) can be written as

$$\Delta B_2 = \nu \overline{f} t^T,$$

where

$$\nu = (t^T s)^{-1}.$$

In view of (6), ΔB_2 minimizes

$$\text{Trace}(\Delta B B^{-1} (\Delta B B^{-1})^T).$$

ΔB_1 and ΔB_2 both approximate the Jacobian, but they differ in what norm they minimize. If $\overline{B}$ is the Jacobian approximation obtained by adding ΔB_1 to B, ΔB_1 is the least change update in the Frobenius norm and ΔB_2 in the weighted Frobenius norm. Using Broyden's update ΔB_1 in Gauss-Newton method shows efficiency on some nonlinear problems, however, in many cases, it does not provide a solution. Since ΔB_2 is an update minimizing in the weighted Frobenius norm with the weight $B^T B$ and the weight is positive definite symmetric matrix, ΔB_2 can be a good candidate for the Jacobian estimate. Nevertheless, if B is ill-conditioned or nearly rank deficient, using $B^T B$ as a weight sometimes shows poor performance. To circumvent this difficulty, we now consider the combination of the two updates

$$(7) \qquad \Delta B = (1-\mu)\Delta B_1 + \mu \Delta B_2,$$

where μ is chosen so that

$$(8) \qquad \| \Delta B_1 \| = \| \mu \Delta B_2 \| .$$

If $y(x_k) = f(x_{k+1}) - f(x_k)$, ΔB in (7) can be written as

$$(9) \qquad \frac{(y_k - B_{k-1}s)s^T}{s^T s}[(1-\mu)I + \frac{tt^T}{t^T t}].$$

By definition in [4], ΔB is an update in the Quasi-Newton class. Now, μ can be decided as follows:

$$\| \Delta B_1 \| = \text{Trace}(\Delta B_1 \Delta B_1^T) = \text{Trace}(\sigma^2 \overline{f} s^T s \overline{f}) = \sigma \overline{f}^T \overline{f},$$

Also,

$$\| \Delta B_2 \| = \text{Trace}(\Delta B_2 \Delta B_2^T) = \text{Trace}(\nu^2 \overline{f} t^T t \overline{f}^T) = \nu^2 \overline{f}^T \overline{f} t^T t,$$

and it follows from (8) that

$$\mu = \frac{\sigma}{\nu^2 t^T t}.$$

Comparison of $Df(x)$ Approximations

The difference between the Jacobian and Broyden's update, denoted by $E_k = B_k - Df(x^*)$, is measured in [3] as follows:

$$\| B_{k+1} - Df(x^*) \| \leq \| B_k - Df(x_k) \| + \frac{\| y - Df(x^*) \|}{\| s \|},$$

where $y_k = f_{k+1} - f_k$. More precisely,

$$\begin{aligned} \| E_{k+1} \|_F &\leq \| E_k (I - \frac{ss^T}{s^T s}) \|_F + \frac{\| (y - Df(x^*) \|_2}{\| s \|_2} \\ &\leq \| E_k \|_F - \frac{1}{2 \| E_k \|_F} \frac{\| E_k s \|^2}{\| s \|^2} + \frac{\| y - Df(x^*) \|_2}{\| s \|_2}. \end{aligned}$$

The difference in the update (7) is determined by the next Theorem.

THEOREM 1. *Let $f : R^n \to R^n$ be a differential function in D, an open convex set. Assume that $Df(x) \in Lip_\gamma(D)$, $B_{k-1} \in R^{n\times n}$, B_k is obtained using (7), and $P = \frac{ss^T}{s^Ts}\{(1-\mu)I + \frac{tt^T}{t^Tt}\}$. If $x^* \in D$ and $Df(x)$ obeys the weaker Lipschitz condition, for either the Frobenius or l_2 matrix norms,*

$$\| Df(x) - Df(x^*) \| \leq \gamma \| x - x^* \|, \text{ for all } x \in D,$$

then,

$$(10) \quad \| B_k - Df(x^*) \|$$
$$\leq \| (B_{k-1} - Df(x^*))(I-P) \| + \frac{\gamma}{2}(\| x_k - x^* \|_2 + \| x_{k-1} - x^* \|_2).$$

Proof. Let $Df^* \equiv Df(x^*)$. Subtracting Df^* from both sides of $B_k = B_{k-1} + \Delta B$ (7),

$$B_k - Df^* = B_{k-1} - Df^* + \frac{(y_k - B_{k-1}s)s^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}].$$

Subtracting and adding $\frac{Df^*s^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}]$ to the right hand side of the above equation,

(11)

$$\begin{aligned} B_k - Df^* &= B_{k-1} - Df^* + \frac{(Df^*s - B_{k-1}s)s^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}] \\ &+ \frac{(y - Df^*s)s^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}] \\ &= (B_{k-1} - Df^*)[I - \frac{ss^T}{s^Ts}\{(1-\mu)I + \frac{tt^T}{t^Tt}\}] \\ &+ \frac{(y - Df^*s)s^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}]. \end{aligned}$$

Now for either the Frobenius or l_2 matrix norm,

$$\begin{aligned} \| B_k - Df^* \| \leq & \| B_{k-1} - Df^*(I-P) \| \\ & + \frac{\| y - Df^*s \|_2}{\| s \|_2} \| P \|_2 . \end{aligned}$$

Since $\| P \|_2 = 1$,

$$\| y - Df^* s \|_2 \leq \frac{\gamma}{2}(\| x_k - x^* \|_2 + \| x_{k-1} - x^* \|_2) \| s \|_2$$

from [6, p. 77], we have (10).

LEMMA 1. *If $s \in R^n$ is nonzero, $E \in R^{n\times n}$, then*

$$\| E(I-P) \|_F \leq \| E \|_F - \frac{1-\mu^2+\mu}{2 \| E \|_F} (\frac{\| Es \|}{\| s \|})^2. \tag{12}$$

Proof. P and $I - P$ satisfy the following equation,

$$\| E \|_F^2 = \| EP \|_F^2 + \| E(I-P) \|_F^2, \tag{13}$$

or,

$$\| E(I-P) \|_F = (\| E \|^2 - \| EP \|^2)^{\frac{1}{2}},$$

and since $\| E \|_F^2 \geq \| EP \|_F^2 \geq 0$, we have

$$\| E(I-P) \|_F \leq \| E \|_F - \frac{1}{2 \| E \|_F} \| EP \|_F^2 . \tag{14}$$

Now,

$$\| EP \|_F^2 = Tr(EPP^T E^T),$$

and

$$\begin{aligned} PP^T &= \frac{ss^T}{s^Ts}[(1-\mu)I + \frac{tt^T}{t^Tt}] \ [(1-\mu)I + \frac{tt^T}{t^Tt}]\frac{ss^T}{s^Ts} \\ &= (1-\mu)^2 \frac{ss^T}{s^Ts} + 2(1-\mu)\frac{ss^Ttt^Tss^T}{(s^Ts)^2t^Tt} + \frac{ss^Ttt^Tss^T}{(s^Ts)^2t^Tt} \\ &= \frac{ss^T}{s^Ts}(1-\mu^2+\mu), \end{aligned}$$

therefore,

$$\begin{aligned} \| EP \|_F^2 &= (1-\mu^2+\mu)Tr(\sigma Ess^TE) \\ &= (1-\mu^2+\mu) \| \sigma Ess^T \|_F^2 \\ &= (1-\mu^2+\mu)\frac{\| Es \|^2}{\| s \|^2}. \end{aligned} \tag{15}$$

Using the above equation in (14), we get (12).

LEMMA 2. *If $s \in R^n$ is nonzero, $E \in R^{n\times n}$, then,*

$$\| E(I-P) \|_F \leq \| E\left(I - \frac{ss^T}{s^Ts}\right) \|_F . \tag{16}$$

Proof. From (13) and (15),

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

and

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

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

$$\| E \|_F^2 - (1-\mu^2+\mu)\left(\frac{\| Es \|}{\| s \|}\right)^2 \leq \| E \|_F^2 - \left(\frac{\| Es \|}{\| s \|}\right)^2$$

which proves (16).

THEOREM 2. *If B_k and $\tilde{B}_k$ are, respectively, the Jacobian estimates obtained using Broyden's update and the update (7), then*

$$\| \tilde{B}_k - Df^* \|_F \leq \| B_k - Df^* \|_F .$$

Proof. Let $E_k = B_k - Df^*$ and $\tilde{E}_k = \tilde{B}_k - Df^*$, then, for Broyden's method, we have

$$\| E_k \|_F \leq \| E_{k-1}(I - \frac{ss^T}{s^Ts}) \|_F + \frac{\| (y_{k-1} - Df^* s^T) \|_2}{\| s \|_2},$$

and for the update (7),

$$\| \tilde{E}_k \|_F \leq \| E_{k-1}(I-P) \|_F + \frac{\| (y_{k-1} - Df^* s^T) \|_2}{\| s \|_2}.$$

In view of Lemma 2, we get $\| \tilde{E}_k \|_F \leq \| E_k \|_F$.

Therefore, we have shown that the update (7) provides better approximate Jacobian than Broyden's. We will use this update in Gauss-Newton method to achieve more accurate results.

3. Gauss-Newton Method

We derive Gauss-Newton methods using Broyden and the combination of updates introduced in the previous section as Jacobian approximations. In Gauss-Newton method [15], instead of solving (3), we solve

$$B^T B s = -B^T f. \tag{17}$$

The Levenberg-Marquardt-Tichonov modification [15] to the above equation of Gauss-Newton method is

$$(B^T B + \epsilon I)s = t,$$

using $-B^T f = t$, where ϵ is a small positive number, say, $\| f \| \cdot 10^{-10}$. The solution s of the above equation minimizes the functional

$$\| Bs + f \|^2 + \epsilon \| s \|^2 .$$

It is recommended in [6] to implement the Levenberg-Marquardt-Tichonov modification rather than plain Gauss-Newton method, we will use the Levenberg-Marquardt-Tichonov modification. Let $W = B^T B$, then (17) becomes

$$Ws = t. \tag{18}$$

For the Levenberg-Marquardt-Tichonov method W is replaced by $W + \epsilon I$. The solution of (18) requires $O(n^3/6)$ operations, since W is symmetric, therefore, only the diagonal and the lower triangular part of W are generated and stored.

Gauss-Newton Method (M3)

If (18) is used in an iterative method it is required to have an updating formula, that is, computing $\overline{W}$ from W. We proceed as follows. If we use Broyden's update and let $\bar{t} = -\overline{B}^T \overline{f}$ and $y = \sigma s$, then

$$\Delta B = \overline{f} y^T, \; \Delta B^T \Delta B = \overline{f}^T \overline{f} y y^T,$$

$$B^T \Delta B = (\overline{B} - \Delta B)^T \Delta B = -\bar{t} y^T - \overline{f}^T \overline{f} y y^T,$$

$$\begin{aligned}\overline{W} &= \overline{B}^T\overline{B} = (B+\Delta B)^T(B+\Delta B)\\ &= B^TB + B^T\Delta B + \Delta B^T B + \Delta B^T\Delta B\\ &= W - \bar{t}y^T - y\bar{t}^T - \overline{f}^T\overline{f}yy^T\\ &= W - (\bar{t} + \overline{f}^T\overline{f}y)y^T - y\bar{t}^T.\end{aligned}$$

Only the diagonal and the lower triangular part of W are stored and updated.

Though the Gauss-Newton method is one of successful methods, it requires stability in solving various problems.

A Proposed Gauss-Newton Method (M4)

To improve Gauss-Newton method, we apply the update (7) to Gauss-Newton method since the update (7) gives the better Jacobian approximation. We also derive a formula to obtain $\overline{W}$ from W.

From (7), we have

$$\Delta B = (1-\mu)\overline{f}y^T + \mu\nu\overline{f}t^T = \overline{f}((1-\mu)y^T + \mu\nu t^T) = \overline{f}z^T,$$

where $z = (1-\mu)y + \mu\nu t$. Furthermore, using

$$\Delta B^T\Delta B = \overline{f}^T\overline{f}zz^T,\ B^T\Delta B = (\overline{B} - \Delta B)^T\Delta B = -\bar{t}z^T - \overline{f}^T\overline{f}zz^T,$$

we have

$$\begin{aligned}\overline{W} &= W - \bar{t}z^T - z\bar{t}^T - \overline{f}^T\overline{f}zz^T\\ &= W - (\bar{t} + \overline{f}^T\overline{f}z)z^T - z\bar{t}^T.\end{aligned}$$

An algorithm for M4 is given as follows:

Algorithm

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

$$W_0 = B_0^T B_0$$

Do for$k = 0, 1, \cdots$:

Solve $W_k s_k = -B_k^T f(x_k)(= t)$ for s_k,

$$x_{k+1} := x_k + s_k,$$

$$z_k := (1-\mu)\frac{s^T}{s^T s} + \mu\nu t^T,$$

$$t_{k+1} := -(B_k + f_{k+1} z_k^T)^T f(x_{k+1}),$$

$$W_{k+1} := W_k - (t_{k+1} + f_{k+1}^T f_{k+1} z) z^T - z t_{k+1}^T.$$

4. Computational Results

Results of computational experiments are summarized in Table 1. The computations were done on Micorvax II. Main set of test problems consists of the nonlinear non-symmetric problems with $f : R^n \to R^n$ listed in ([12], [13]), which are usually used to evaluate new algorithms [11]. They include Extended Rosenbrook function, Extended Powell singular function, Trigonometric function, Brown's almost linear function, Discrete internal equation, Broyden tridiagoanl function, and Broyden's banded function. Test for robustness with respect to poor scaling were also implemented by modifying our test set as $f(x) = f(\Sigma x)$ where Σ is a diagonal matrix with poorly scaled entries. Initial Jacobians were evaluated numerically by finite differences. In order to improve inconsistency of Gauss-Newton method mentioned in [8] for various problems, we mainly investigated average time of the problems for the methods. From Table 1, M4 is significantly better than all the other methods and its performance improves with the increase in the size of the problems. For example, Broyden's method (M1) took 125% more and Gauss-Newton (M3) 112% more than M4 for $n = 80$. Furthermore, M4 failed only in four cases as compared to 9 for Gauss-Newton method (M3) and 17 for Broyden's method (M1). On some problem, M3 performed better than others however, it failed to get a solution more often than M2 and M4. which indicates lack of reliability of M3. The relative efficiency of M3 and M4 is due to the fact that W is symmetric and only $O(n^3/6)$ operations were needed to solve (18) as compared to $O(n^3/3)$ required to solve (3) in M1 and M2. We found and M4 were more robust than M1, M2 and M3 when n was large.

Size	M1	M2	M3	M4
n=20	1.55	1.31	1.03	1.00
n=40	1.75	1.52	1.07	1.00
n=80	2.25	1.69	1.12	1.00
Average for All Sizes	1.86	1.51	1.12	1.00
Number of cases of Non-Convergence/Divergence	17	6	9	4

Table 1:Average relative times for all methods with method 4 as the basis.

References

1. C. G. Broyden, *A Class of Methods for Solving Nonlinear Simultaneous Equations*, Math. Comp. **19** (1969), 577–593.
2. C. G. Broyden, *Quasi-Newton Methods and Their Application to Function Minimization*, Math. Comp. **21** (1967), 76–90.
3. J. E. Dennis and J. J. Moré, *A Characterization of Superlinear Convergence and Its Application to Quasi-Newton Methods*, Math. Comp. **28** (1974), 549–560.
4. J. E. Dennis and J. J. Moré, *Quasi-Newton Methods, motivation and theory*, SIAM Review **19** (1977), 46–89.
5. J.E. Dennis and R.B. Schnabel, *Least Change Updates for Quasi-Newton Methods*, SIAM Review **21** (1979), 443–459.
6. J. E. Dennis and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Prentice-Hall Inc., Englewood Cliffs, New Jersey, 1983.
7. L. C. Dixon,, *Quasi-Newton Algorithm Generates Identical Points*, Math. Comp. **3** (1972), 345–358.
8. C. Fraley,, *Computational behavior of Gauss-Newton Methods*, SIAM J. Sci. Stat. Comput. **10 No. 3** (1989), 515–532.
9. D. M. Gay,, *Computing Optimal Locally Constrained steps*, SIAM J. Sci. Stat. Comput. **2** (1981), 186–197.
10. P. E. Gill and W. Murray, and M. H. Wright, *Practical Optimization*, Academic Press, London, 1981.
11. K. L. Hilbert, *An Evaluation of Mathematical Software That Solves Systems of Nonlinear Equations*, ACM Tran. Math. Soft. **8 No. 1** (1982), 5–20.

12. J. J. Moré, B. S. Garbow, and K. E. Hillstrom, *Fortran Subroutines for Testing Unconstrained Optimization Software*, TOMS **7** (1981), 136–140.
13. J. J. Moré, B. S. Garbow, and K. E. Hillstrom, *Testing Unconstrained Optimization Software*, ACM Trans. Math. Software **7** (1981), 17–41.
14. J. Stoer and R Bulirsch, *Numerical Analysis*, Springer-Verlag, New York, 1980.
15. R. P. Tewarson, *Use of Smoothing and damping techniques in the solution of nonlinear equations*, SIAM Rev **19** (1977), 35–45.

Department of Mathematics
Ewha Women's University
Suhdaemoon-gu, Seoul, Korea