An improved quasi-Newton equation on the quasi-Newton methods for unconstrained optimizations

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ABSTRACT

Quasi-Newton methods are a class of numerical methods for solving the problem of unconstrained optimization. To improve the overall efficiency of resulting algorithms, we use the quasi-Newton methods which is interesting for quasi-Newton equation. In this manuscript, we present a modified BFGS update formula based on the new quasi-Newton equation, which give a new search direction for solving unconstrained optimizations proplems. We analyse the convergence rate of quasi-Newton method under some mild condition. Numerical experiments are conducted to demonstrate the efficiency of new methods using some test problems. The results indicates that the proposed method is competitive compared to the BFGS methods as it yielded fewer iteration and fewer function evaluations.

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1. INTRODUCTION

Quasi-Newton method is one of the main iterative methods designed to solve unconstrained optimization problem [1]. The method has the (1).

$$Min \quad f(x) \ , \ x \in \mathbb{R}^n \tag{1}$$

where $f: \mathbb{R}^n \to \mathbb{R}$, is smooth function. More details can be found in [2]. The iterative method takes the (2).

$$x_{k+1} = x_k + \alpha_k d_k \tag{2}$$

where α_k is the parameter determined by exact line-search as.

$$\alpha_k = -\frac{g_k^T d_k}{d_k^T Q d_k} \tag{3}$$

More details can be found in [3]. The search direction d_k generated by.

$$B_k d_k + g_k = 0 \tag{4}$$

where B_k is an approximation of the Hessian matrix [4]. In this manuscript, we pay attention to the BFGS method in which B_k is updated by (5).

$$B_{k+1}^{BFGS} = B_k - \frac{B_k s_k s_k^T B_k^T}{s_k^T B_k s_k} + \frac{y_k y_k^T}{s_k^T y_k}$$
(5)

where $s_k = x_{k+1} - x_k = \alpha_k d_k$ and $y_k = g_{k+1} - g_k$. Consider H_k be the inverse of B_k . Surely, the (5) update can be written as (6).

$$H_{k+1}^{BFGS} = H_k - \frac{H_k y_k s_k^T + s_k y_k^T H_k}{s_k^T y_k} + \left[1 + \frac{y_k^T H_k y_k}{s_k^T y_k}\right] \frac{s_k s_k^T}{s_k^T y_k}$$
(6)

To the best of our knowledge the BFGS method may fail to converge by using Wolfe line search for non-convex optimization and also by using with exact line search constructed Dai [2] and Mascarenhas [5]. To defeat (remedy) this case, quasi-Newton equation has been modified in some way or other can be seen some formulas among others as.

Author(s)	QN – conditions	References
Wei, Li, and Qi	$B_{k+1}s_k = y_k = y_k + \frac{2(f_k - f_{k+1}) + (g_{k+1} + g_k)^T s_k}{s_k^T v_k} v_k$	[6]
Biglari, Hassan, and Leon	$B_{k+1}s_k = y_k = y_k + \frac{4(f_k - f_{k+1}) + 2(g_{k+1} + g_k)^T s_k}{s_k^T v_k} v_k$	[7]
Chen, Deng, and. Zhang	$B_{k+1}s_k = y_k = y_k + \frac{6(f_k - f_{k+1}) + 3(g_{k+1} + g_k)^T s_k}{s_k^T v_k} v_k$	[8]
Basim	$B_{k+1}s_k = \bar{y}_k = \frac{1}{2}y_k + \frac{(f_k - f_{k+1}) - 1/2(g_{k+1}^T s_k)}{s_k^T v_k}v_k$	[9]
Basim and Mohammed	$B_{k+1}s_k = \tilde{y}_k = y_k - \frac{g_{k+1}^T s_k}{s_k^T U_k} U_k$	[10]
Basim and Ghada	$B_{k+1}s_{k} = \tilde{y_{k}} = y_{k} + \frac{2(f_{k} - f_{k+1}) - s_{k}^{T}y_{k}}{s_{k}^{T}\upsilon_{k}}\upsilon_{k}$	[11]

where v_k is any vector satisfying $s_k^T v_k \neq 0$. In [12], a general framework of modified methods is proposed to solve non-convex optimization problems. Thus the modifying methods can guarantee the updated matrix is positive definite which guarantees a descent direction. The convergent properties are also established and generated more accurate second-order curvature approximations than the usual quasi-Newton updates do.

The quasi-Newton equation plays an important role, on studies some of the quasi-Newton methods. In this paper, we propose a modification to the hessian matrix Bk resulting in a new quasi-newton method based on new quasi-Newton equation. The proposed method can guarantee that the updated matrix is positive definite which guarantees a descent direction. The convergent properties are also established. More so the proposed method generates a more accurate second-order curvature approximations than the usual quasi-Newton updates.

2. DERIVING THE NEW QUASI-NEWTON EQUATION

Zahra and Ali [13] propose a type quasi-Newton equation of quasi-Newton methods and generate several QN directions, as (7).

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$$\nabla^2 f(x_{k+1}) s_k = \tilde{y}_k = y_k + \frac{5}{3} \frac{\max\left\{2(f_k - f_{k+1}) + (g_{k+1} + g_k)^T s_k, 0\right\}}{s_k^T v_k} v_k$$
(7)

For more details can be found in [13].

So we will deriving quasi-Newton equation motivated by quasi-Newton (7). Now multiplying it by s_k^T , we have.

$$s_{k}^{T} \nabla^{2} f(x_{k+1}) s_{k} = s_{k}^{T} \tilde{y}_{k} = s_{k}^{T} y_{k} + \frac{5}{3} \left\{ 2(f_{k} - f_{k+1}) + (g_{k+1} + g_{k})^{T} s_{k} \right\}$$
(8)

we can write:

$$\frac{3}{5}s_k^T \nabla^2 f(x_{k+1})s_k = \frac{3}{5}s_k^T y_k + 2(f_k - f_{k+1}) + (g_{k+1} + g_k)^T s_k$$
(9)

Now, from (3) and (9), we obtain.

$$s_{k}^{T}\nabla^{2}f(x_{k+1})s_{k} = \frac{3}{5}s_{k}^{T}y_{k} + 2(f_{k} - f_{k+1}) + (g_{k+1} + g_{k})^{T}s_{k} + \frac{2}{5}s_{k}^{T}\nabla^{2}f(x_{k+1})s_{k}$$

$$s_{k}^{T}\nabla^{2}f(x_{k+1})s_{k} = \frac{3}{5}s_{k}^{T}y_{k} + 2(f_{k} - f_{k+1}) + (g_{k+1} + g_{k})^{T}s_{k} - \frac{2}{5}g_{k}^{T}s_{k}$$
(10)

From (10) we get.

$$s_{k}^{T} \nabla^{2} f(x_{k+1}) s_{k} = \frac{3}{5} s_{k}^{T} y_{k} + 2(f_{k} - f_{k+1}) + g_{k+1}^{T} s_{k} + \frac{3}{5} g_{k}^{T} s_{k}$$
(11)

Consider B_{k+1} is an approximate of the Hessian matrix $\nabla^2 f(x_{k+1})$ of the $f(x_k)$.

$$s_k^T B_{k+1} s_k = \frac{3}{5} s_k^T y_k + 2(f_k - f_{k+1}) + g_{k+1}^T s_k + \frac{3}{5} g_k^T s_k$$
(12)

This gives a new quasi-Newton equation in the form.

$$B_{k+1}s_k = y_k = \frac{3}{5}y_k + \frac{2(f_k - f_{k+1}) + g_{k+1}^T s_k + 3/5g_k^T s_k}{s_k^T v_k}v_k$$
(13)

where v_k is any vector satisfying $s_k^T v_k \neq 0$. Motivated by the idea of Zahra and Ali [8], we propose a modified above quasi-Newton equation, we get as.

$$B_{k+1}s_k = y_k = \frac{3}{5}y_k + \frac{\max\left\{2(f_k - f_{k+1}) + g_{k+1}^T s_k + 3/5g_k^T s_k\right\}}{s_k^T v_k}v_k$$
(14)

Obviously two choices for \mathcal{U}_k can be computed as.

1. First case $v_k = g_{k+1}$ gives:

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$$B_{k+1}s_{k} = y_{k}^{*} = \frac{3}{5}y_{k} + \frac{\max\left\{2(f_{k} - f_{k+1}) + g_{k+1}^{T}s_{k} + 3/5g_{k}^{T}s_{k}\right\}}{s_{k}^{T}g_{k+1}}g_{k+1}$$
(15)

2. Second case $v_k = y_k$ gives:

$$B_{k+1}s_k = y_k^* = \frac{3}{5}y_k + \frac{\max\left\{2(f_k - f_{k+1}) + g_{k+1}^T s_k + 3/5g_k^T s_k\right\}}{s_k^T y_k}y_k$$
(16)

Using quasi-Newton equation in the BFGS update to give a good result. Now, we are in a situation to explain our algorithm in details.

Stage 1. Give \mathcal{E} , a initial point $x_0 \in \mathbb{R}^n$. Set k = 0.

- Stage 2. If possible test satisfies then stop.
- **Stage 3.** Solve $B_k d_k = -g_k$.

Stage 4. Find α_k by using the following Wolfe conditions :

$$f(x_k + \alpha_k d_k) \le f(x_k) + \delta \alpha_k g_k^T d_k$$
(17A)

$$d_k^T g(x_k + \alpha_k d_k) \ge \sigma \, d_k^T g_k \tag{17B}$$

where $0 < \delta < \sigma < 1$.

Stage 5. Set $x_{k+1} = x_k + \alpha_k d_k$. Compute y_k^* by (14). If $s_k^T y_k^* > 0$, update H_{k+1} by (6), otherwise let $H_{k+1} = H_k$. Set k = k+1 and go to Step 2.

The major work, we introduce the positive definite property for the new quasi-Newton equation.

Theorem 1.

Suppose that $s_k^T y_k > 0$. Then B_{k+1} is symmetric positive definite.

Proof.

Using definition y_k and multiplying by s_k^T , we get:

$$s_{k}^{T} y_{k}^{*} = \frac{3}{5} s_{k}^{T} y_{k} + 2(f_{k} - f_{k+1}) + g_{k+1}^{T} s_{k} + \frac{3}{5} g_{k}^{T} s_{k}$$
(18)

From (19), (17) and (18), we obtained.

$$s_{k}^{T} y_{k}^{*} \geq -2\delta g_{k}^{T} s_{k} + \frac{8}{5} \sigma g_{k}^{T} s_{k}$$

$$\geq -2\sigma g_{k}^{T} s_{k} + \frac{8}{5} \sigma g_{k}^{T} s_{k}$$

$$\geq -\frac{2}{5} \sigma g_{k}^{T} s_{k}$$
(19)

As $s_k^T g_k = \alpha_k d_k^T g_k < 0$, then

$$s_k^T y_k > -2/5\sigma \alpha_k d_k^T g_k \tag{20}$$

Denote the right side part of the inequality by Λ , then one has.

 $s_k^T y_k^* > \Lambda > 0 \tag{21}$

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So B_{k+1} is positive definite.

Though the $s_k^T y_k > 0$, does not hold true for non-convex problems, B_{k+1} may not be positive definite. It serves as a useful condition for positive definiteness of the updates consider.

$$K = \left\{ k : \frac{s_k^T y_k}{\|s_k\|^2} \ge \beta \|g_k\|^{\delta} \right\},$$
(22)

where $\beta > 0$ is constant and $\delta > 0$ is bounded.

3. CONVERGENCE ANALYSIS

We will study the global convergence of our method. We need some assumptions. Let the level set $D = \{x \mid f(x) \le f(x_0)\}\$, with x_0 is an initial point of iterative method is restricted.

Using Lipschitz continuous; that is exist constants L and γ , such that.

$$\left\|\nabla f(\upsilon) - \nabla f(\omega)\right\| \le L \left\|\upsilon - \omega\right\|, \quad \forall \ \upsilon, \ \omega \in D$$
⁽²³⁾

and,

$$\left\|\nabla f(x)\right\| \le \gamma \ , \ \forall \ x \in D \tag{24}$$

Since $\{f(x_k)\}$ is a no increasing, which ensures $\{x_k\}$ is contained in D and the existence of x^* we have.

$$\lim_{k \to \infty} f(x_k) = f(x^*) \tag{25}$$

Moreover, from the fact that sequence x_k is bounded, there exists μ , such that $\forall k$,.

$$\|s_{k}\| = \|x - \bar{x}\| \le \|x\| + \|\bar{x}\| \le \mu$$
(26)

More details can be found in [14], [15].

Presented the useful theorem to prove that our method is globally convergent.

Theorem 2.

If $\|\nabla f(x)\| \le \gamma$ is not satisfies for all k. Let $\{x_k\}$ be generated by modified methods, and the (27) holds.

$$\|B_k s_k\| \le a_1 \|s_k\|$$
 and $s_k^T B_k s_2 \ge a_2 \|s_k\|^2$, (27)

where $a_1 > 0$ and $a_2 > 0$ are constants. For infinitely k, then we have.

$$\lim_{k \to \infty} \inf \|g_k\| = 0 \tag{28}$$

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By (4) of the Wolfe conditions we obtain.

$$(g_{k+1} - g_k)^T d_k \ge -(1 - \sigma)g_k^T d_k$$
⁽²⁹⁾

By using Lipschitz condition we obtain.

$$(g_{k+1} - g_k)^T d_k \le L\alpha_k \|d_k\|$$
(30)

This implies that.

$$\alpha_{k} \geq \frac{-(1-\sigma)g_{k}^{T}d_{k}}{L\|d_{k}\|^{2}} = \frac{(1-\sigma)d_{k}^{T}B_{k}d_{k}}{L\|d_{k}\|^{2}} \geq \frac{(1-\sigma)a_{2}}{L}$$
(31)

using (22) we obtain.

$$\sum_{k=1}^{\infty} (f_k - f_{k+1}) = \lim_{N \to \infty} \sum_{k=1}^{\infty} (f_k - f_{k+1}) = \lim_{N \to \infty} (f_1 - f_{k+1}) = f_1 - f^*$$
(32)

The (32) implies

$$\sum_{k=1}^{\infty} (f_k - f_{k+1}) \le + \infty,$$
(33)

This together with Wolfe condition (3) yields.

$$\sum_{k=1}^{\infty} -\alpha_k g_k^T d_k \le +\infty$$
(34)

Then

$$\lim_{k \to \infty} \alpha_k g_k^T d_k = 0 \tag{35}$$

in cooperation with (31) provide that.

$$\lim_{k \to \infty} d_k^T B_k d_k = \lim_{k \to \infty} -g_k^T d_k = 0$$
(36)

Combining (33) with (24) we obtain the conclusion (25). The proof is finished.

Nevertheless, we give the lemma for large scale problems to show the convergence property for new algorithm. This lemma was shown by Powell [16].

Lemma 1.

If BFGS method with Wolfe condition is applied to a continuously differentiable function f that is bounded below, and if there exists a constant M such that the inequality holds.

$$\frac{\left\|\boldsymbol{y}_{k}\right\|^{2}}{\boldsymbol{s}_{k}^{T} \boldsymbol{y}_{k}} \leq \boldsymbol{M}$$
(37)

Then,

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$$\lim_{k \to \infty} \inf \|g_k\| = 0 \tag{38}$$

Theorem 3.

Let $\{x_k\}$ be generated by the proposed method and $v_k \leq \chi \|s_k\|$. Then we have.

$$\lim_{k \to \infty} \inf \|g_k\| = 0 \tag{39}$$

Proof:

Using a contradiction method with there exists $\varepsilon > 0$ such that.

$$\|\boldsymbol{g}_k\| > \boldsymbol{\varepsilon} \tag{40}$$

Hence, (22) imply that.

$$s_{k}^{T} y_{k}^{*} \ge \beta \left\| g_{k} \right\|^{\delta} \left\| s_{k} \right\|^{2} \ge \beta \gamma^{\delta} \left\| s_{k} \right\|^{2}$$

$$\tag{41}$$

By the definition of y_k can be written as.

$${}^{*}_{k} = \frac{3}{5} y_{k} + \frac{\varpi_{k}}{s_{k}^{T} \upsilon_{k}} \upsilon_{k}, \quad \varpi_{k} = \max\left\{0, 2(f_{k} - f_{k+1}) + g_{k+1}^{T} s_{k} + 3/5 g_{k}^{T} s_{k}\right\}$$
(42)

So, from (24), we get.

$$y_{k}^{*T} y_{k}^{T} = \frac{9}{25} (Gs_{k})^{2} + \frac{6}{5} (Gs_{k}) \frac{\overline{\sigma}_{k}}{s_{k}^{T} \upsilon_{k}} \upsilon_{k} + (\frac{\overline{\sigma}_{k}}{s_{k}^{T} \upsilon_{k}})^{2} \upsilon_{k}^{T} \upsilon_{k}$$
(43)

By simple computation and using $\upsilon_k \leq \chi \| s_k \|$, we obtain,

$$\left\| \overset{*}{\boldsymbol{y}}_{\boldsymbol{k}} \right\|^{2} \leq \boldsymbol{s}_{\boldsymbol{k}}^{T} \left(\frac{3}{5} \boldsymbol{G} + \boldsymbol{\chi} \frac{\boldsymbol{\varpi}_{\boldsymbol{k}}}{\boldsymbol{s}_{\boldsymbol{k}}^{T} \boldsymbol{\upsilon}_{\boldsymbol{k}}} \right)^{2} \boldsymbol{s}_{\boldsymbol{k}} \leq \boldsymbol{\nu} \left\| \boldsymbol{s}_{\boldsymbol{k}} \right\|^{2}$$

$$\tag{44}$$

Therefore, by dividing the sides of inequalitie $\left\| y_k \right\|^2$, inequalities (41) we obtain.

$$\frac{\left\|\begin{array}{c}y_{k}\\y_{k}\end{array}\right\|^{2}}{s_{k}^{T}y_{k}} \leq M$$
(45)

Using lemma 1, to the sub $\{B_k\}_{k \in K}$, obviously, clearly there exist a_1 and a_2 we get (27) for infinitely many k. Then theorem 2. complete the proof.

4. NUMERICAL REPORTS

In this part, we details results of some numerical experiments with the new method and algorithm BFGS. We choose 30 test problems with the different dimension and initial points from literature [17]. Some enlargement was observed for class from test problems [18]-[24]. We set the parameters $\sigma_1 = 0.1$, $\sigma_2 = 0.9$ and $\varepsilon = 10^{-5}$ in the numerical experiment. By applying law Himmeblau [25], the stop criterion is "If

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 $|f(x_k)| > 10^{-5}$, let $stop \ 1 = |f(x_k) - f(x_{k+1})| / |f(x_k)|$; Otherwise, let $stop \ 1 = |f(x_k) - f(x_{k+1})|$. For every problem, if $||g_k|| < \varepsilon$ or $stop \ 1 < 10^{-5}$ is satisfied, the program will be stopped". The numerical results based on IN and NF, the number of iterations and the number of function evaluations, respectively.

A comparison of the algorithms is given based on the performance profiles of Dolan and More [26]. The comparison is based on NI and NF, respectively. The plots obtained via the Dolan and More performance profiles indicate that the M2 and M3 methods perform better than the M1 method. To facilitate this, we used the following notations to represent the algorithms: M1. This is the standard BFGS method defined by (6). M2. This is the new algorithm with $v_{t} = y_{t}$ is used. M3. This is defined by (17) with using $v_{t} = g_{t+1}$. Figure 1 and Figure 2, we have found that new proposed methods best BFGS method in about (17-53)% NI and (49-51)% NF. The new methods has good numerical results.



Figure 1. Number of iteration profile via dolan and more



Figure 2. Number of function evaluation profile via dolan and more profile

5. CONCLUSIONS

The paper studies the quasi-Newton method which is popular in solving large-scale unconstrained optimization. It presents a new quasi-Newton equation for gradient methods. Numerical comparisons with the well-known BGGS method are given. Inspired new quasi-Newton very well in practice in comparison with quasi-Newton methods.

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