A modified BFGS method and its convergence

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Abstract

In this paper, a new modified BFGS method for unconstrained optimization problems is presented. The algorithm preserves the convergence properties of the famous BFGS algorithm. The relation between the new algorithm and a self-scaling quasi-Newton algorithm is revealed. If we assume the objective function is twice continuously differentiable and uniformly convex, we prove the iteration converge globally to the solution. And under some additional conditions, the superlinear convergence is given. Finally, the experimental results show that the proposed algorithm performs very well, which indicate that the numerical performance of the new algorithm is somewhat like the self-scaling quasi-Newton algorithm.

Keywords: modified BFGS method, convergence, unconstrained problems

1 Introduction

In this paper, we consider the following unconstrained optimization problems. See Equation (1).

$$\min f(x), x \in \mathbf{R}^n, \tag{1}$$

where $f: R^n \to R$ is continuously differentiable. The BFGS method is a well-known quasi-Newton method for solving unconstrained problems. During the past two decades, the study on global convergence of the quasi-Newton method has received growing interests. When f is convex, it was shown that Broyden's class of quasi-Newton methods converge globally if exact line search is used [1].When inexact line search is used, Powell [2] first obtained the global convergence of BFGS method. Byrd, Nocedal and Yuan [3] extended Powell's results to the restricted Broyden's class of quasi-Newton methods with Wolfe-Type line search except for DFP method. Yuan [4] and Wei [5] proposed modified secant equations which approximate the curvature of the objective function more accurate than the standard secant equation. On the other hand, in order to solve the nonconvex problems, Li and Fukushima [6] made a slight modification to the standard BFGS method.

Recently, Lewis and Overton [7] have shown in numerical experiments that the standard BFGS method works very well when applied directly without modifications to nonsmooth test problems as long as a weak Wolfe line search is used. All the mentioned methods in [3, 4, 5, 6] use both the gradient and function values available at the current iteration. In the cases that the Hessian matrix has some special structures and is partially available. For example, in the nonlinear least squares problems, the above mentioned secant equations have been developed by Amini and Ghorbani Rizi [8]. Xiao [9] proposed a modified limited memory BFGS method for solving the unconstrained. Saman [10] proposed two effective hybrid conjugate gradient algorithms based on modified BFGS updates. In the paper, we will analysis how to form the approximate matrix and how to use the formed approximate matrix to replace the inverse of the Hessian matrix in the BFGS method. Compared to the traditional BFGS method, the modified BFGS is also well-defined.

BFGS requires only matrix-vector multiplications which brings the computational cost at each iteration from O (n^3) for Newton's method down to O (n^2). However, if the number of variables is very large, even O (n^2) per iteration is too expensive - both in terms of CPU time and sometimes also in terms of memory usage (a large matrix must be kept in memory at all times). According to the idea of Li and Fukushima. In the paper a modified BFGS method for unconstrained problems is applied even if the number of variables is very large. The modified BFGS method can save computing time.

The organization of this paper is as follows. In the next section we shall describe the new modified BFGS algorithm. If we assume the objective function is twice continuously differentiable and uniformly convex, according to the idea of Byrd, in section 3 we prove the iteration converge globally to the solution, and in section 4 under some additional conditions we show the method is superlinearly convergent. In section 5 the numerical results of the algorithm is shown. Finally, we make conclusions in section 6.

2 The new modified BFGS method

For brevity, we first introduce some notations used in this paper: $g_k = g(x_k), g = \nabla f$ gradient of f ; $G = \nabla^2 f$

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Hessian matrix of f ; d_k, λ_k, search vector/step length; $s_k = x_k - x_{k-1}, y_k = g_k - g_{k-1}$.

With $\|\cdot\|$ we will denote the Euclidean vector norm in R^n, as well as the corresponding operator norm of matrices in $\mathbf{R}^{n\times n}$.

Algorithm 2.1(the new modified BFGS method)

Step1: Choose an initial point $x_1 \in \mathbf{R}^n$ and an initial positive definite matrix $\mathbf{B}_1$, and positive constants α, β with $0<\alpha<0.5, \alpha<\beta<1$. Let $k=0$.

Step2: If $g_k = 0$, stop; otherwise, go to Step3.

Step3: For given $x_k, \mathbf{B}_k$, solve the system of linear equation $\mathbf{B}_k d_k + g_k = 0$ to obtain a unique optimal solution d_k.

Step4: Compute λ_k, which satisfies

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k s_k s_k^{\mathbf{T}} \mathbf{B}_k}{s_k^{\mathbf{T}} \mathbf{B}_k s_k} + \frac{y_k y_k^{\mathbf{T}}}{y_k^{\mathbf{T}} s_k}, \quad (4)$$

where $y_k = \begin{cases} \bar{y}_k \\ \bar{y}_k + (c\|g_k\| - \frac{\bar{y}_k s_k}{\|s_k\|^2}) \end{cases}$,

$$\text{if } \; y_k^{\mathbf{T}} s_k \geq c\|g_k\|\|s_k\|^2, \quad \text{else} \quad (5)$$

$$\bar{y}_k = g_{k+1} - g_k + r_k s_k, \quad (6)$$

and

$$r_k = \frac{3(g_{k+1}+g_k)^{\mathbf{T}} s_k - 6(f_{k+1}-f_k)}{\|s_k\|^2} \quad (7)$$

then set $k=k+1$, go to Step2.

3 Global convergence

In this section, we study the global convergence of algorithm2.1.First we make the following assumptions:
(1): The level set $D=\{x \mid f(x) \leq f(x_0)\}$ is contained in a bounded convex set D.
(2): The objective function f is continuously differentiable on D and there is a constant $L>0$ such that for any $x, y \in D$,

$$\|g(x)-g(y)\| \leq L\|x-y\|. \quad (8)$$

(3): The function f is uniformly convex, i.e., there exist two positive constants m and M such that

$$m\|z\|^2 \leq z^{\mathbf{T}} G(x) z \leq M\|z\|^2 \quad (9)$$

for all $z \in \mathbf{R}^n$ and all $x \in D$.

Lemma 3.1 Suppose the sequence $\{x_k\}$ is generated by Alorithm 2.1.Then we have for every $k=0,1,\cdots$, $f(x_{k+1}) - f(x_k) < 0$.

Proof: For any positive definite matrix $\mathbf{B}_{k-1}$, from (2) we get $f(x_{k+1}) - f(x_k) \leq \alpha\lambda_k g_k^{\mathbf{T}} d_k = -\alpha\lambda_k d_k^{\mathbf{T}} \mathbf{B}_{j-1} d_k < 0$, it implies that the new iteration point belongs to D. Due to (3) we also have

$$y_k^{\mathbf{T}} d_{k-1} = (g_k - g_{k-1}) d_{k-1} \geq -(\beta-1) d_{k-1}^{\mathbf{T}} \mathbf{B}_{j-1} d_{k-1} > 0. \quad (10)$$

Since $s_k = \lambda_{k-1} d_{k-1}$, from (10) we get $y_k^{\mathbf{T}} s_k > 0$, this indicates that Alorithm 2.1 has the property if $\mathbf{B}_{k-1}$ is symmetric positive definite, then $\mathbf{B}_k$ is also symmetric positive definite.

Lemma 3.2 Let the sequence $\{x_k\}$ is generated by Alorithm 2.1.Suppose the assumption hold. Then we can get

$$\|y_k\| \leq \max\{7L, 7L + cC_1\}\|s_k\|, k=1,2,\ldots. \quad (11)$$

Proof: By using (5), if $\bar{y}_k^{\mathbf{T}} s_k \geq c\|g_k\|\|s_k\|^2$, we have $y_k = \bar{y}_k$. Therefore, $\|y_k\| \leq \|g_{k+1} - g_k\| + |r_k|\|s_k\|$, from the (8), we have

$$y_k \leq (L + |r_k|)\|s_k\|, \quad (12)$$

where $|r_k| = \frac{|3(g_{k+1}-g_k)^{\mathbf{T}} s_k - 6(f_{k+1}-f_k)|}{\|s_k\|^2}$.

From the Taylor's formula, we get

$$|r_k| \leq \frac{|3(g_k + \theta_1 s_k) - g_{k+1} + 3(g_k + \theta_1 s_k) - g_k|}{\|s_k\|^2} \leq 6L. \quad (13)$$

Substitute (13) into (12), we can get $\|y_k\| \leq 7L\|s_k\|, k=1,2,\ldots$.

In the other hand, if $y_k = g_{k+1} - g_k + r_k + c\|g_k\| - \frac{\bar{y}_k^{\mathbf{T}} s_k}{\|s_k\|^2} s_k$, using the Taylor's formula and (8), we also get $\|y_k\| \leq \|g_{k+1} - g_k\| + |r_k| + c(\|g_k\| + \frac{\|\bar{y}_k^{\mathbf{T}} s_k\|}{\|s_k\|^2})\|s_k\|$

$\leq (7L + c\|g_k\|)\|s_k\|$.

According to the assumption (1), there exists a positive constant C_1, $\|g_k\| \leq C_1$, thus, we have $\|y_k\| \leq (7L + cC_1)\|s_k\|$.

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Lemma 3.3 Let the sequence $\{x_k\}$ is generated by Alorithm 2.1. Suppose $\mathbf{B}_0$ is symmetric positive definite.

Then there is a constant $H \geq 0$ for all $k \geq 1$, y_k and s_k satisfy

$$\frac{\|y_k\|^2}{y_k^{\mathrm{T}} s_k} \leq H, \quad (14)$$

Consequently, for any $p \in (0,1)$ there exist positive constants $\beta_1, \beta_2, \beta_3$ such that, for $k \geq 1$ the following inequality

$$\beta_2 \leq \frac{\|\mathbf{B}_j s_j\|}{\|s_j\|} \leq \frac{\beta_3}{\beta_1} \equiv \beta. \quad (15)$$

Proof: Using Lemma 3.2, we can easily get $\frac{\|y_k\|^2}{y_k^{\mathrm{T}} s_k} \leq \frac{\max\{7L, 7L + cC_1\}\|s_k\|}{\|s_k\|}$.

Therefore, we have $\frac{\|y_k\|^2}{y_k^{\mathrm{T}} s_k} \leq H$, where $H = \max\{7L, 7L + cC_1\}$. From the theorem 2.1 in [11], we get (15).

Our proof is completed.

We defined set $K = \{k \mid k$ satisfies (15)$\}$.

Thus, from the right hand of (15), we have

$$\|\mathbf{B}_k s_k\| \leq \beta \|s_k\|, \quad k \in K. \quad (16)$$

Moreover, for all $k \in K$, $\|\mathbf{B}_k s_k\| = |\lambda_k| \|\mathbf{B}_k d_k\| = |\lambda_k| \|g_k\| \leq \beta \|s_k\| = \beta |\lambda_k| \|d_k\|$.

So we can get

$$\|g_k\| \leq \beta \|d_k\|. \quad (17)$$

By using $y_k = \mathbf{B}_k s_k$ and (9), we have

$$m\|s_k\|^2 \leq \|s_k^{\mathrm{T}} \mathbf{B}_k s_k\| \leq M \|s_k\|^2, \quad (18)$$

where m and M are positive constants.

There m 3.4 Let the sequence $\{x_k\}$ is generated by Alorithm 2.1.Suppose the assumption hold. Then we get

$$\liminf_{k\to\infty} \|g_k\| = 0. \quad (19)$$

Proof: We firstly assume $\|g_k\| \geq \varepsilon$ for all $k \in K$ with positive constant ε. Using Lemma 3.1, (16), (18) and $\mathbf{B}_k s_k = \lambda_k \mathbf{B}_k d_k = -\lambda_k g_k$, we can get

$$+\infty \geq \sum_{k=0}^{\infty} (-g_k^{\mathrm{T}} s_k) = \sum_{k=0}^{\infty} \frac{1}{\lambda_k} s_k^{\mathrm{T}} \mathbf{B}_k s_k = \sum_{k=0}^{\infty} \lambda_k \frac{\|g_k\|^2}{\|\mathbf{B}_k s_k\|^2} s_k^{\mathrm{T}} \mathbf{B}_k s_k$$
$$\geq \sum_{k=0}^{\infty} \frac{\|g_k\|^2}{\|\mathbf{B}_k s_k\|^2} s_k^{\mathrm{T}} m \|s_k\|^2 \geq \sum_{k=0}^{\infty} \beta^{-2} m \|g_k\|^2 \geq \sum_{k=0}^{\infty} \beta^{-2} m \varepsilon^2 = \infty.$$

It is obvious that we have derived a contradiction, so (19) holds.

The above theorem is established the global convergence of Alorithm 2.1.

4 Superlinear convergence

In order to give the superlinear convergence of Algorithm 2.1, we also need the following assumptions. Let x^* be the limit of the sequence $\{x_k\}$.

(4): f is twice continuously differentiable for all x in the neighbourhood of x^*.

(5): $\{x_k\}$ converges to x^*, where $g(x^*) = 0$ and $G(x^*)$ is positive definite.

(6): There exist two constants $M_2 \geq 0$ and $v \geq 0$ such that

$$\|G(x) - G(x^*)\| \leq M_2 \|x - x^*\|^v. \quad (20)$$

Lemma 4.1 Suppose assumptions (4)-(6) hold. Let us define θ_k as the angle between s_k and $\mathbf{B}_k s_k$. According to Byrd [3], it follows that $\cos\theta_k = \frac{s_k^{\mathrm{T}} \mathbf{B}_k s_k}{\|s_k\| \|\mathbf{B}_k s_k\|}$, so we get

$$a_1 \|g_k\| \cos\theta_k \leq \|s_k\|, \quad (21)$$

where a_1 is a positive constant.

Proof: From the assumption (2) and the definition y_k, we obtain

$$y_k s_k^{\mathrm{T}} \geq c\|g_k\|\|s_k\|^2 \geq c\|s_k\|(-g_k^{\mathrm{T}} s_k) \geq c\varepsilon_0(-g_k^{\mathrm{T}} s_k). \quad (22)$$

Combining assumption (4) and assumption (2), we have $\|G(x)\| \leq M_1$, $\|g(x)\| \leq M_2$, with M_1 and M_2 are a positive constants.

So we get

$$M_1\|s_k\|^2 \geq \|G(\varepsilon_1)s_k\|\|s_k\| = \|g_{k+1} - g_k\|\|s_k\| \geq y_k s_k^{\mathrm{T}}$$
$$\geq c\varepsilon_0(-g_k^{\mathrm{T}} s_k) = c\varepsilon_0 \|g_k\|\|s_k\|\cos\theta_k, \quad (23)$$

where $\varepsilon_1 = x_k + \delta s_k, \delta \in (0,1)$.

(23) implies (22) holds, where $a_1 = \frac{c\varepsilon_0}{M}$.

Lemma 4.2 If the assumptions (1)-(6) hold, for an arbitrary $v > 0$, we can obtain

$$\sum_{k=0}^{\infty} \|x_{k+1} - x_k\|^v < +\infty, \quad (24)$$

and

$$\sum_{k=0}^{\infty} r_k < +\infty, \quad (25)$$

where $r_k = \max\{\|x_{k+1} - x^*\|^v, \|x_k - x^*\|^v\}$.

Proof: By the assumption (4) and (5), we have the following inequality

$$\|g(x)\| = \|g(x) - g(x^*)\| \geq m_1 \|x - x^*\|, \quad (26)$$

where m_1 is a positive constant.

From (15) and Lemma 4.1, we have

$$\cos\theta_k \geq 1/\beta. \quad (27)$$

Therefore,

$$\begin{aligned} -g_k^{\mathrm{T}} s_k &= \|g_k\| \|s_k\| \cos\theta_k \geq a_1 \|g_k\| \cos^2\theta_k \\ &\geq a_1 m_1^2 \|x_k - x^*\| \cos^2\theta_k \\ &\geq a_1 m^2 \frac{1}{\beta} \|x_k - x^*\|^2 \end{aligned} \quad (28)$$

By (2), (3) and (28), we can get (24).It is obvious that (25) hold.

Theorem 4.3 Let $\{\mathbf{B}_k\}$ and $\{x_k\}$ be generated by Alorithm 2.1, f satisfies assumption (4)-(6), then for any $k \geq 0$, we can get

(1): $$\lim_{k\to\infty} \frac{\|(\mathbf{B}_k - G(x^*))s_k\|}{\|s_k\|} = 0, \quad (29)$$

(2): $\{x_k\}$ generated by Alorithm 2.1 superlinearly converges to x^*.

Proof: By using Lemma 4.1 and Lemma 4.2, we can easily obtain (29).Similar to the arguments of Dennis [11], we get

$$\lim_{k\to\infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0. \quad (30)$$

5 Numerical experiments

In this section we present the results of our numerical experiments to compare the algorithm suppose by Broyden in [1] and the algorithm 2.1 in this paper. For brevity, we use BFGS and MBFGS to represent the algorithm suppose by Broyden in [1] and the algorithm 2.1 in this paper. All the numerical experiments will be programmed by matlab2012b. Let us choose the same starting point for both BFGS and MBFGS. In algorithm 2.1, while $c = 10^{-3}$, $\alpha = 0.3, \beta = 0.8$, $\mathbf{B}_0 = E$, and the experiment is stop when $\|g\| \leq 10^{-5}$.

(i) Problem 1. $f(x) = x_1^4 + x_2^4 + 2x_1^2 x_2^2 - 4x_1 + 3$,

(ii) Problem 2. $f(x) = (x_1 + x_2)^2 + [2(x_1^2 + x_2^2 - 1) - \frac{1}{3}]^2$,

(iii). Problem 3. (Rosenbrock's function, $n = 2$) $f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$

(iv). Problem 4 (Cube function, $n = 2$) $f(x) = 100(x_2 - x_1^3)^2 + (1 - x_1)^2$

Please see Table 1.

TABLE 1 Numerical results of BFGS and MBFGS methods

Test Functions	Initial points	n_i		n_f		x^*	f^*
		BFGS	**MBFGS**	**BFGS**	**MBFGS**		
(i)	(1.25,1.25)	8	5	41	26	(1,0)	0
	(12,12)	8	6	41	31		
	(45,45)	8	6	41	31		
(ii)	(-1.25,0.5)	8	6	41	31	(0.763756, 0.763679)	0
	(-1.25,-1)	13	9	62	42		
	(-1.25,1)	7	5	35	26		
(iii)	(-10,10)	30	12	151	61	(1,1)	0
	(10,-10)	68	23	341	156		
	(100,100)	167	25	836	235		
(iv)	(10,10)	52	18	46	31	(1,1)	0
	(30,80)	75	23	61	42		
	(-15,15)	28	19	72	32		

In Table 1, n_i and n_f indicates the number of iteration and the number of function evaluation respectively. Meanwhile, x^* and f^* indicates minimum points and minimum value respectively. It can be seen from the comparison given above that the algorithm 2.1 in this paper is more efficient than BFGS method for solving unconstrained optimization.

6 Conclusions

In this paper, a modified BFGS algorithm for unconstrained problems is proposed. If we assume the objective function is twice continuously differentiable and uniformly convex, we prove the iteration converge globally to the solution. And under some additional conditions the superlinear convergence is given. The method retains the scale-invariance property of the original BFGS method. We have preliminary numerical results to show its efficiency. As demonstrated in Section 5, the reported numerical results show that the modified BFGS performs better than the BFGS in [1].

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