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A modified BFGS method and its global convergence in nonconvex minimization

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Abstract

In this paper, we propose a modification of the BFGS method for unconstrained optimization. A remarkable feature of the proposed method is that it possesses a global convergence property even without convexity assumption on the objective function. Under certain conditions, we also establish superlinear convergence of the method. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Let $f:\mathbb{R}^n \to \mathbb{R}$ be continuously differentiable. Consider the following unconstrained optimization problem:

$$\min f(x), \quad x \in \mathbb{R}^n. \tag{1.1}$$

Throughout the paper, we assume that the objective function f in (1.1) has Lipschitz continuous gradients, i.e., there is a constant $L > 0$ such that

$$\|g(x) - g(y)\| \leqslant L\|x - y\|, \quad \forall x, y \in \mathbb{R}^n, \tag{1.2}$$

where $g(x)$ denotes the gradient of f at x and $\|\cdot\|$ denotes the Euclidean norm of a vector. We will often abbreviate $g(x_k)$, $f(x_k)$, etc. as g_k, f_k, etc., respectively.

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Among numerous iterative methods for solving (1.1), quasi-Newton methods constitute a particularly important class. During the past two decades, global convergence of quasi-Newton methods has received growing interests. When f is convex, it was shown that Broyden's class of quasi-Newton methods converges globally and superlinearly if exact line search is used (see [12,6]). When inexact line search is used, Byrd et al. [3] proved global and superlinear convergence of the convex Broyden's class with Wolfe-type line search except for DFP method. Byrd and Nocedal [2] obtained global convergence of BFGS method with backtracking line search. Zhang and Tewarson [15] obtained global convergence of the preconvex Broyden's class of methods. Li [11] proved that when f is a convex quadratic function, DFP method still retains global convergence. There are many other studies on global convergence of quasi-Newton methods (see, e.g., [9,13,14]). We refer to Fletcher [8] for a recent review.

We note that these studies focused on the case where the function f is convex. What will happen if quasi-Newton methods are applied to (1.1) where f is not convex? Under what conditions does BFGS method converge globally and superlinearly for nonconvex minimization problems? These questions have remained open for many years (see [7,8]). The purpose of this paper is to study these problems. We will show that if BFGS method is slightly modified, then under suitable conditions, the modified method converges globally and superlinearly even for nonconvex unconstrained optimization problems.

We organize the paper as follows. In the next section, we give the motivation of our study and describe the modified method. In Section 3, we discuss global convergence and superlinear convergence of the modified method with Wolf-type line search. In Section 4, we describe a practicable modified BFGS method and establish its global and superlinear convergence. In Section 5, we extend the results obtained in Section 4 to the algorithm with backtracking line search.

2. Motivation and algorithm

In this section, we present a modified BFGS method after describing our motivation.

First, we briefly review Newton's method. Suppose for the moment that f is twice differentiable. Then Newton's method for solving (1.1) takes the following iterative process. Given the kth iterate x_k, we determine the Newton direction p_k by

$$G_k p_k + g_k = 0, \tag{2.1}$$

where $G_k = G(x_k)$ denotes the Hessian matrix of f at x_k. Once p_k is obtained, the next iterate is generated by $x_{k+1} = x_k + p_k$. Under suitable conditions, Newton's method converges locally and quadratically. To enlarge the convergence domain of Newton's method, a globalization strategy may be employed. In particular, when G_k is positive definite, the vector p_k determined by (2.1) is a descent direction of f at x_k. Thus, one can choose a step length $\lambda_k > 0$ satisfying

$$f(x_k + \lambda_k p_k) \leqslant f(x_k) + \sigma \lambda_k g(x_k)^{\mathrm{T}} p_k, \tag{2.2}$$

where $\sigma \in (0,1)$ is a given constant. Line search (2.2) can be fulfilled by a backtracking process of Armijo-type, i.e., $\lambda_k = \rho^{i_k}$, where $\rho \in (0,1)$ is a given constant and i_k is the smallest nonnegative integer i for which $\lambda_k = \rho^i$ satisfies (2.2). Then the next iterate is given by $x_{k+1} = x_k + \lambda_k p_k$. Newton's method with line search is called a damped Newton method. It converges globally and quadratically under some conditions.

Quasi-Newton methods were developed based on Newton's method, in which G_k is substituted by some matrix B_k to avoid the calculation of a Hessian matrix. That is, Newton direction is approximated by the so-called quasi-Newton direction p_k generated by

$$B_k p_k + g_k = 0, \tag{2.3}$$

where B_k is an approximation of $G(x_k)$. Among various quasi-Newton methods, BFGS method is currently regarded as the most efficient method. In this method, B_k is updated by the following formula:

$$B_{k+1} = B_k - \frac{B_k s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}, \tag{2.4}$$

where $s_k = x_{k+1} - x_k$ and $\gamma_k = g_{k+1} - g_k$. The update formula (2.4) has the property that if B_k is symmetric positive definite and $\gamma_k^{\mathrm{T}} s_k > 0$, then B_{k+1} is also symmetric positive definite. Therefore the quasi-Newton direction p_k generated by (2.3) is a descent direction of f at x_k no matter whether G_k is positive definite or not.

Convergence properties of BFGS method have been well studied on convex minimization problems (see, e.g., [2,3,12–14]). Yet it is not known whether this method converges globally when it is applied to nonconvex minimization problems even if exact line search is used. Moreover, since $G(x)$ is generally not positive definite when f is nonconvex, there seems no reason to believe that a positive definite B_k still affords a good approximation of G_k. So, it would be reasonable to expect that a proper modification of the method is effective for nonconvex problems.

Recall that in the case where f is nonconvex, the Newton direction p_k generated by (2.1) may not be a descent direction of f at x_k since G_k is not necessary positive definite. Therefore the line search (2.2) may not be well-defined. To overcome this difficulty, Newton's method has been modified in some way or other. For example, we may generate a direction p_k from (2.1) in which G_k is replaced by the matrix

$$\bar{G}_k \triangleq G_k + r_{k-1} I, \tag{2.5}$$

where I is the unit matrix and a positive constant r_{k-1} is chosen so that $\bar{G}_k$ is positive definite. For this modified Newton's method, we have the following result.

Theorem 2.1. *Let the level set*

$$\Omega = \{x \mid f(x) \leqslant f(x_0)\}$$

be bounded and f be twice continuously differentiable on a convex set containing Ω. Assume that $\{x_k\}$ is generated by the modified Newton's method using matrices $\bar{G}_k$ given by (2.5) *and Armijo-type line search satisfying* (2.2). *Suppose that $\{r_k\}$ is bounded above and that there exists an accumulation point $\bar{x}$ of $\{x_k\}$ with $G(\bar{x})$ being positive definite. Then the following statements hold*:

(i) *We have*

$$\liminf_{k \to \infty} \|g_k\| = 0. \tag{2.6}$$

(ii) *If we assume further that $\{x_k\} \to \bar{x}$, $r_k \to 0$, and $\sigma \in (0, \frac{1}{2})$, then the convergence rate is at least superlinear.*

(iii) *If in addition, $G(x)$ is Lipschitz around $\bar{x}$ and there exists a constant $C>0$ such that $r_{k-1}\leqslant C\|g_k\|$ for all k, then the convergence rate is quadratic.*

Proof. (i) Summing inequalities (2.2), we obtain

$$-\sum_{k=0}^{\infty}\sigma\lambda_k g_k^{\mathrm{T}}p_k\leqslant f(x_0)-\lim_{k\to\infty}f(x_k)<\infty,$$

where the limit exists because of the descent property of $\{f(x_k)\}$ and the boundedness of Ω. In particular, $\lambda_k g_k^{\mathrm{T}}p_k\to 0$. Let $\{x_k\}_{k\in K}\to\bar{x}$ on some subsequence. Denote $\bar{\lambda}=\liminf_{k\to\infty,\,k\in K}\lambda_k\geqslant 0$. If $\bar{\lambda}>0$, then $g_k^{\mathrm{T}}p_k\to 0$ or equivalently $-g_k^{\mathrm{T}}\bar{G}_k^{-1}g_k\to 0$ as $k\to\infty$ with $k\in K$. Since $G(\bar{x})$ is positive definite and $r_k\geqslant 0$ for each k, $\{\bar{G}(x_k)\}_{k\in K}$ is uniformly positive definite when k is sufficiently large. Then it is easy to deduce that $\|g(\bar{x})\|=\lim_{k\in K,\,k\to\infty}\|g_k\|=0$.

If $\bar{\lambda}=0$, without loss of generality, we assume that $\lim_{k\in K,k\to\infty}\lambda_k=0$ and $\bar{G}_k\to\bar{G}(\bar{x})$ as $k\to\infty$ with $k\in K$, where the latter particularly follows from the boundedness of $\{r_k\}$. By the line search criterion, when $k\in K$ is sufficiently large, $\lambda_k'\triangleq\lambda_k/\rho$ does not satisfy (2.2). In other words, we have

$$f(x_k+\lambda_k'p_k)-f(x_k)>\sigma\lambda_k'g(x_k)^{\mathrm{T}}p_k.$$

Dividing by λ_k' and taking limits in both sides as $k\to\infty$ we get

$$g(\bar{x})^{\mathrm{T}}\bar{p}\geqslant\sigma g(\bar{x})^{\mathrm{T}}\bar{p}, \tag{2.7}$$

where $\bar{p}=-\bar{G}(\bar{x})^{-1}g(\bar{x})$. Since $G(\bar{x})$ is positive definite and r_k is nonnegative, it is clear that both $\bar{G}(\bar{x})$ and $\bar{G}(\bar{x})^{-1}$ are positive definite. Since $\sigma\in(0,1)$, (2.7) implies that $g(\bar{x})^{\mathrm{T}}\bar{p}=-g(\bar{x})^{\mathrm{T}}\bar{G}(\bar{x})^{-1}g(\bar{x})\geqslant 0$. It then follows that $g(\bar{x})=0$, i.e., (2.6) holds.

(ii) By assumption, we have $p_k=-\bar{G}(x_k)^{-1}g_k\to 0$. Since $r_k\to 0$, we have

$$\begin{aligned}f(x_k+p_k)-f(x_k)-\sigma g_k^{\mathrm{T}}p_k&=(1-\sigma)g_k^{\mathrm{T}}p_k+\tfrac{1}{2}p_k^{\mathrm{T}}G(x_k)p_k+o(\|p_k\|^2)\\&=-(1-\sigma)p_k^{\mathrm{T}}\bar{G}(x_k)p_k+\tfrac{1}{2}p_k^{\mathrm{T}}G(x_k)p_k+o(\|p_k\|^2)\\&=-(1-\sigma-\tfrac{1}{2})p_k^{\mathrm{T}}\bar{G}(x_k)p_k-\tfrac{1}{2}p_k^{\mathrm{T}}(\bar{G}(x_k)-G(x_k))p_k+o(\|p_k\|^2)\\&=-(\tfrac{1}{2}-\sigma)p_k^{\mathrm{T}}\bar{G}(x_k)p_k+o(\|p_k\|^2),\end{aligned}$$

where the last equality follows from the assumption $r_k\to 0$. Since $\sigma\in(0,\frac{1}{2})$ and $\bar{G}(x_k)$ is positive definite, it follows that when k is sufficiently large, the unit stepsize $\lambda_k\equiv 1$ is accepted by the line search criterion. Thus $x_{k+1}=x_k+p_k$ for all k large enough. Moreover, we have

$$\begin{aligned}0&=\bar{G}_kp_k+g_k\\&=\bar{G}_k(x_k+p_k-\bar{x})+g_k-\bar{G}_k(x_k-\bar{x})\\&=\bar{G}_k(x_{k+1}-\bar{x})+g(x_k)-g(\bar{x})-G_k(x_k-\bar{x})-r_{k-1}(x_k-\bar{x})\\&=\bar{G}_k(x_{k+1}-\bar{x})+\left[\int_0^1G(\bar{x}+t(x_k-\bar{x}))\,\mathrm{d}t-G_k\right](x_k-\bar{x})-r_{k-1}(x_k-\bar{x}).\end{aligned}$$

That is,

$$x_{k+1}-\bar{x}=-\bar{G}_k^{-1}\left[\int_0^1 G(\bar{x}+t(x_k-\bar{x}))\,\mathrm{d}t-G_k\right](x_k-\bar{x})-r_{k-1}\bar{G}_k^{-1}(x_k-\bar{x}).$$

Since $G(\bar{x})$ is positive definite and $r_k \geqslant 0, \bar{G}_k$ is uniformly positive definite for sufficiently large k. Thus, we deduce from the above equality that there exists a positive constant M such that

$$\|x_{k+1}-\bar{x}\| \leqslant M\left\{\int_0^1 \|G(\bar{x}+t(x_k-\bar{x}))-G_k\|\,\mathrm{d}t+r_{k-1}\right\}\|x_k-\bar{x}\|, \tag{2.8}$$

which proves (ii).

(iii) From (2.8) we have that

$$\begin{aligned}\|x_{k+1}-\bar{x}\| &\leqslant M\left\{\int_0^1 \|G(\bar{x}+t(x_k-\bar{x}))-G_k\|\,\mathrm{d}t+r_{k-1}\right\}\|x_k-\bar{x}\|\\ &\leqslant M\left\{\int_0^1 \|G(\bar{x}+t(x_k-\bar{x}))-G_k\|\,\mathrm{d}t+C\|g_k\|\right\}\|x_k-\bar{x}\|\\ &= M\left\{\int_0^1 \|G(\bar{x}+t(x_k-\bar{x}))-G_k\|\,\mathrm{d}t+C\|g(x_k)-g(\bar{x})\|\right\}\|x_k-\bar{x}\|\\ &\leqslant M(L_1+CL)\|x_k-\bar{x}\|^2,\end{aligned}$$

where $L>0$ and $L_1>0$ are Lipschitz constants of g and G, respectively. □

The above theorem shows that if we choose r_k in a suitable way (practicable choice of r_k will be discussed in Section 4), then the modified damped Newton's method still retains fast local convergence as well as global convergence. This fact prompts us to consider the following question: Is it possible to modify quasi-Newton methods in such a way that B_k approximates $\bar{G}_k$, thereby ensuring global and superlinear convergence without convexity assumption on the problem?

To answer this question, first observe that since G_{k+1} satisfies

$$G_{k+1}(x_{k+1}-x_k)\approx g_{k+1}-g_k,$$

the matrix $\bar{G}_{k+1}$ will satisfy the relation

$$\bar{G}_{k+1}(x_{k+1}-x_k)=(G_{k+1}+r_kI)(x_{k+1}-x_k)\approx(g_{k+1}-g_k)+r_k(x_{k+1}-x_k)$$

or equivalently

$$\bar{G}_{k+1}s_k\approx\gamma_k+r_ks_k, \tag{2.9}$$

where $\gamma_k=g_{k+1}-g_k$. Therefore, it would be reasonable to require the matrix B_{k+1} to satisfy (2.9) exactly, i.e.,

$$B_{k+1}s_k=y_k, \tag{2.10}$$

where $y_k = \gamma_k + r_k s_k$. If r_k is small, (2.10) can be regarded as an approximation of the ordinary secant equation $B_{k+1}s_k = \gamma_k$.

Now, we propose a modified BFGS method based on the above consideration.

Algorithm 1 (Modified BFGS method: MBFGS).

Step 0: Choose an initial point $x_0 \in \mathbb{R}^n$ and an initial positive-definite matrix B_0. Choose constants σ_1, σ_2 and C such that $0 < \sigma_1 < \sigma_2 < 1$ and $C > 0$. Let $k := 0$.

Step 1: Solve the following linear equation to get p_k:

$$B_k p + g_k = 0.$$

Step 2: Find a stepsize $\lambda_k > 0$ satisfying the Wolfe-type line search conditions:

$$\begin{aligned} &f(x_k + \lambda_k p_k) \leqslant f(x_k) + \sigma_1 \lambda_k g_k^{\mathrm{T}} p_k, \\ &g(x_k + \lambda_k p_k)^{\mathrm{T}} p_k \geqslant \sigma_2 g_k^{\mathrm{T}} p_k. \end{aligned} \tag{2.11}$$

Moreover, if $\lambda_k = 1$ satisfies (2.11), we take $\lambda_k = 1$.

Step 3: Let the next iterate be $x_{k+1} = x_k + \lambda_k p_k$.

Step 4: Let $s_k = x_{k+1} - x_k = \lambda_k p_k$, $\gamma_k = g_{k+1} - g_k$, $\eta_k = \gamma_k^{\mathrm{T}} s_k / \|s_k\|^2$ and $y_k = \gamma_k + r_k s_k$, where $r_k \in [0, C]$.

Step 5: Update B_k using the formula

$$B_{k+1} = B_k - \frac{B_k s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k}. \tag{2.12}$$

Step 6: Let $k := k + 1$ and go to Step 1.

3. General convergence analysis

We begin with the global convergence analysis of MBFGS method. It is easy to see that if λ_k satisfies (2.11), then B_{k+1} is symmetric positive definite provided that B_k is symmetric positive definite. We also notice that the Lipschitz continuity of g ensures that

$$|\eta_k| = \frac{|\gamma_k^{\mathrm{T}} s_k|}{\|s_k\|^2} \leqslant \frac{\|\gamma_k\|}{\|s_k\|} \leqslant L, \quad k = 1, 2, \ldots .$$

This together with Step 4 of Algorithm 1 implies

$$\eta_k + r_k \leqslant L + C, \quad k = 1, 2, \ldots . \tag{3.1}$$

In other words, $\{\eta_k + r_k\}$ is bounded from above. To establish global convergence of Algorithm 1, the lower boundedness of $\{\eta_k + r_k\}$ is also necessary. That is, we need throughout this section that

$$\eta_k + r_k \geqslant \varepsilon, \quad k = 1, 2, \ldots, \tag{3.2}$$

holds for some constant $\varepsilon > 0$. We will show in Section 4 that inequality (3.2) is satisfied by a proper choice of r_k.

In the remainder of the paper, we always assume that the level set

$$\Omega = \{x \mid f(x) \leqslant f(x_0)\}$$

is bounded. It is clear from the first inequality of (2.11) that $\{f(x_k)\}$ is a nonincreasing sequence, which ensures that $\lim_{k\to\infty} f(x_k)$ exists and $\{x_k\} \subset \Omega$.

To establish the global convergence of MBFGS method, we first prove some useful lemmas.

Lemma 3.1. *Let $\{x_k\}$ be generated by MBFGS method. Then we have*

$$\sum_{k=0}^{\infty} (-g_k^{\mathrm{T}} s_k) < \infty, \tag{3.3}$$

$$\varepsilon \|s_k\|^2 \leqslant y_k^{\mathrm{T}} s_k \leqslant (L+C)\|s_k\|^2, \quad k = 1,2,\ldots, \tag{3.4}$$

$$\|y_k\| \leqslant (L+C)\|s_k\|, \quad k = 1,2,\ldots, \tag{3.5}$$

where C and ε are as specified in the Algorithm 1 *and* (3.2), *and L is the Lipschitz constant of g given by* (1.2).

Proof. Since f is bounded below, (3.3) can be obtained by summing the first inequalities of (2.11). Inequalities (3.4) and (3.5) follow from (3.1) and (3.2). □

Lemma 3.2. *There is a constant $M_1 > 0$ such that*

$$\operatorname{tr} B_{k+1} \leqslant M_1(k+1) \quad \textit{and} \quad \sum_{i=0}^{k} \frac{\|B_i s_i\|^2}{s_i^{\mathrm{T}} B_i s_i} \leqslant M_1(k+1). \tag{3.6}$$

Proof. By Lemma 3.1, taking the trace operation on both sides of (2.12) yields

$$\begin{aligned}
\operatorname{tr} B_{k+1} &= \operatorname{tr} B_k - \frac{\|B_k s_k\|^2}{s_k^{\mathrm{T}} B_k s_k} + \frac{\|y_k\|^2}{y_k^{\mathrm{T}} s_k} \\
&\leqslant \operatorname{tr} B_k - \frac{\|B_k s_k\|^2}{s_k^{\mathrm{T}} B_k s_k} + \frac{(L+C)^2}{\varepsilon} \\
&\;\;\vdots \\
&\leqslant \operatorname{tr} B_0 - \sum_{i=0}^{k} \frac{\|B_i s_i\|^2}{s_i^{\mathrm{T}} B_i s_i} + \frac{(L+C)^2}{\varepsilon}(k+1).
\end{aligned}$$

Since B_{k+1} is positive definite, $\operatorname{tr} B_{k+1} > 0$. The last inequality implies (3.6). □

Lemma 3.3. *There is a constant $c > 0$ such that for k all sufficiently large*,

$$\prod_{i=0}^{k} \lambda_i \geqslant c^k. \tag{3.7}$$

Proof. Taking the determinant in (2.12) we get

$$
\begin{aligned}
\det B_{k+1} &= \det\left(B_k\left(I - \frac{s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{B_k^{-1} y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k}\right)\right)\\
&= \det B_k \det\left(I - s_k \frac{(B_k s_k)^{\mathrm{T}}}{s_k^{\mathrm{T}} B_k s_k} + B_k^{-1} y_k \frac{y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k}\right)\\
&= \det B_k \left[\left(1 - s_k^{\mathrm{T}} \frac{B_k s_k}{s_k^{\mathrm{T}} B_k s_k}\right)\left(1 + (B_k^{-1} y_k)^{\mathrm{T}} \frac{y_k}{y_k^{\mathrm{T}} s_k}\right) - \left(-s_k^{\mathrm{T}} \frac{y_k}{y_k^{\mathrm{T}} s_k}\right)\left(\frac{(B_k s_k)^{\mathrm{T}}}{s_k^{\mathrm{T}} B_k s_k} B_k^{-1} y_k\right)\right]\\
&= \det B_k \frac{y_k^{\mathrm{T}} s_k}{s_k^{\mathrm{T}} B_k s_k}\\
&\geqslant \det B_k \frac{\gamma_k^{\mathrm{T}} s_k}{s_k^{\mathrm{T}} B_k s_k}\\
&\geqslant \det B_k \frac{-(1-\sigma_2) g_k^{\mathrm{T}} s_k}{-\lambda_k g_k^{\mathrm{T}} s_k}\\
&= \frac{1-\sigma_2}{\lambda_k} \det B_k\\
&\;\vdots\\
&\geqslant \left(\prod_{i=0}^{k} \frac{1}{\lambda_k}\right)(1-\sigma_2)^{k+1} \det B_0,
\end{aligned}
$$

where the third equality follows from the formula (see, e.g., [5, Lemma 7.6])

$$
\det(I + u_1 u_2^{\mathrm{T}} + u_3 u_4^{\mathrm{T}}) = (1 + u_1^{\mathrm{T}} u_2)(1 + u_3^{\mathrm{T}} u_4) - (u_1^{\mathrm{T}} u_4)(u_2^{\mathrm{T}} u_3)
$$

and the second inequality follows from the second inequality of (2.11).

Since $\det B_{k+1} \leqslant ((1/n)\mathrm{tr}\, B_{k+1})^n \leqslant ((1/n)M_1(k+1))^n$ by Lemma 3.2, we deduce from the above inequality that

$$
\prod_{i=0}^{k} \lambda_k \geqslant \frac{(1-\sigma_2)^{k+1} \det B_0}{\det B_{k+1}} \geqslant \frac{(1-\sigma_2)^{k+1} \det B_0}{((1/n)M_1(k+1))^n}.
$$

When k is sufficiently large, this implies (3.7). □

Now we establish a global convergence theorem for MBFGS method. The proof is similar to the one given in [14].

Theorem 3.4. *Let* $\{x_k\}$ *be generated by MBFGS method with* B_k *being updated by* (2.12). *Then we have*

$$
\liminf_{k\to\infty} \|g_k\| = 0. \tag{3.8}
$$

Proof. For the purpose of contradiction we assume that $\|g_k\| \geqslant \gamma > 0$ for all k. Since $B_k s_k = \lambda_k B_k p_k = -\lambda_k g_k$, it follows from (3.3) that

$$\begin{aligned}
\infty &> \sum_{k=0}^{\infty} (-g_k^{\mathrm{T}} s_k) \\
&= \sum_{k=0}^{\infty} \frac{1}{\lambda_k} s_k^{\mathrm{T}} B_k s_k \\
&= \sum_{k=0}^{\infty} \frac{\|g_k\|}{\|B_k s_k\|}\, s_k^{\mathrm{T}} B_k s_k \\
&= \sum_{k=0}^{\infty} \|g_k\|^2 \lambda_k \, \frac{s_k^{\mathrm{T}} B_k s_k}{\|B_k\ s_k\|^2} \\
&\geqslant \gamma^2 \sum_{k=0}^{\infty} \lambda_k \, \frac{s_k^{\mathrm{T}} B_k s_k}{\|B_k s_k\|^2}.
\end{aligned}$$

Therefore, for any $\zeta > 0$, there exists an integer $k_0 > 0$ such that for any positive integer q,

$$q \left(\prod_{k=k_0+1}^{k_0+q} \lambda_k \frac{s_k^{\mathrm{T}} B_k s_k}{\|B_k s_k\|^2} \right)^{1/q} \leqslant \sum_{k=k_0+1}^{k_0+q} \lambda_k \frac{s_k^{\mathrm{T}} B_k s_k}{\|B_k s_k\|^2} \leqslant \zeta,$$

where the left-hand inequality follows from the geometric inequality. Thus

$$\begin{aligned}
\left(\prod_{k=k_0+1}^{k_0+q} \lambda_k \right)^{1/q} &\leqslant \frac{\zeta}{q} \left(\prod_{k=k_0+1}^{k_0+q} \frac{\|B_k s_k\|^2}{s_k^{\mathrm{T}} B_k s_k} \right)^{1/q} \\
&\leqslant \frac{\zeta}{q^2} \sum_{k=k_0+1}^{k_0+q} \frac{\|B_k s_k\|^2}{s_k^{\mathrm{T}} B_k s_k} \\
&\leqslant \frac{\zeta}{q^2} \sum_{k=0}^{k_0+q} \frac{\|B_k s_k\|^2}{s_k^{\mathrm{T}} B_k s_k} \\
&\leqslant \frac{\zeta(k_0 + q + 1)}{q^2} M_1.
\end{aligned}$$

Letting $q \to \infty$ yields a contradiction, because Lemma 3.3 ensures that the left-hand side of the above inequality is greater than a positive constant. Thus, we get (3.8). □

The above theorem shows a global convergence property of MBFGS method without convexity assumption on f. It only relies on the assumption that f has Lipschitz continuous gradients.

Now we turn to establishing a superlinear convergence property of MBFGS method.

To do this, we need the following set of assumptions.

Assumption (A). (1) f is twice continuously differentiable near x^*.

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

(3) G is Hölder continuous at x^*, i.e., there exist constants $v > 0$ and $M_2 > 0$ such that

$$\|G(x) - G(x^*)\| \leqslant M_2 \|x - x^*\|^v \tag{3.9}$$

for all x in a neighborhood of x^*.

(4) $\{r_k\}$ satisfies

$$\sum_{i=0}^{\infty} r_k < \infty. \tag{3.10}$$

Under conditions (1) and (2) in Assumption (A), there is a neighbourhood $U(x^*)$ of x^* such that $G(x)$ is uniformly positive definite for all $x \in U(x^*)$. Therefore, there is a constant $m > 0$ such that for all $x \in U(x^*)$

$$\|g(x)\| = \|g(x) - g(x^*)\| \geqslant m\|x - x^*\| \tag{3.11}$$

and

$$d^{\mathrm{T}} G(x) d \geqslant m\|d\|^2 \quad \text{for all } d \in \mathbb{R}^n. \tag{3.12}$$

In particular, (3.11) and (3.12) hold with $x = x_k$ for all k sufficiently large.

Let ϕ_k denote the angle between s_k and $B_k s_k$, i.e.,

$$\cos\phi_k = \frac{s_k^{\mathrm{T}} B_k s_k}{\|s_k\|\,\|B_k s_k\|} = -\frac{g_k^{\mathrm{T}} s_k}{\|g_k\|\,\|s_k\|}.$$

We will establish superlinear convergence of MBFGS method after proving several lemmas similar to those in [3].

Lemma 3.5. *Under conditions* (1) *and* (2) *in Assumption* (A), *there are constants $a_1 > 0$, $a_1' > 0$ and $a_2 > 0$ and an index k' such that when $k \geqslant k'$*,

$$a_1'\|g_k\|\cos\phi_k \leqslant \|s_k\| \leqslant a_1\|g_k\|\cos\phi_k, \tag{3.13}$$

$$\prod_{i=0}^{k} \cos^2\phi_i \geqslant a_2^{k+1}. \tag{3.14}$$

Proof. From (2.11) and Taylor's expansion with (3.12), there is an index k_1 such that when $k \geqslant k_1$

$$\sigma_1 g_k^{\mathrm{T}} s_k \geqslant f_{k+1} - f_k \geqslant g_k^{\mathrm{T}} s_k + \frac{m}{2}\|s_k\|^2,$$

which implies that

$$\|s_k\|^2 \leqslant -\frac{2(1-\sigma_1)}{m} g_k^{\mathrm{T}} s_k = \frac{2(1-\sigma_1)}{m}\|g_k\|\,\|s_k\|\cos\phi_k.$$

Letting $a_1 = 2(1-\sigma_1)/m$, we get the right-hand inequality of (3.13).

Again by (2.11) and (3.4) we have

$$(L + C)\|s_k\|^2 \geqslant y_k^{\mathrm{T}} s_k \geqslant \gamma_k^{\mathrm{T}} s_k \geqslant -(1-\sigma_2) g_k^{\mathrm{T}} s_k = (1-\sigma_2)\|g_k\|\,\|s_k\|\cos\phi_k.$$

Letting $a_1' = (1-\sigma_2)/(L+C)$ yields the left-hand inequality of (3.13).

Since $\|B_k s_k\| = \lambda_k \|g_k\|$, (3.13) implies that when $k \geqslant k_1$

$$\frac{\|B_k s_k\|^2}{s_k^T B_k s_k} = \frac{\|B_k s_k\|}{\|s_k\| \cos\phi_k} = \frac{\lambda_k \|g_k\|}{\|s_k\| \cos\phi_k} \geqslant \frac{\lambda_k}{a_1 \cos^2\phi_k}.$$

Multiplying these inequalities from k_1 to $k > k_1$ and using the geometric inequality, we get

$$\begin{aligned}
\left(\prod_{i=k_1}^{k} \frac{\lambda_i}{a_1 \cos^2\phi_i}\right)^{1/(k-k_1+1)} &\leqslant \left(\prod_{i=k_1}^{k} \frac{\|B_i s_i\|^2}{s_i^T B_i s_i}\right)^{1/(k-k_1+1)} \\
&\leqslant \frac{1}{k-k_1+1} \sum_{i=k_1}^{k} \frac{\|B_i s_i\|^2}{s_i^T B_i s_i} \\
&\leqslant \frac{1}{k-k_1+1} \sum_{i=0}^{k} \frac{\|B_i s_i\|^2}{s_i^T B_i s_i} \\
&\leqslant M_1 \frac{k+1}{k-k_1+1},
\end{aligned}$$

where the last inequality follows from (3.6). Therefore we obtain for any k large enough

$$\begin{aligned}
\prod_{i=k_1}^{k} \cos^2\phi_i &\geqslant \left(\prod_{i=k_1}^{k} \lambda_i\right) a_1^{-(k-k_1+1)} M_1^{-(k-k_1+1)} \left(\frac{k-k_1+1}{k+1}\right)^{k-k_1+1} \\
&= \left(\prod_{i=0}^{k} \lambda_i\right) a_1^{-(k-k_1+1)} M_1^{-(k-k_1+1)} \left(\frac{k-k_1+1}{k+1}\right)^{k-k_1+1} \prod_{i=0}^{k_1-1} \lambda_i^{-1} \\
&\geqslant c^k \left(a_1^{-1} M_1^{-1} \frac{k-k_1+1}{k+1}\right)^{k-k_1+1} \prod_{i=0}^{k_1-1} \lambda_i^{-1},
\end{aligned}$$

where the last inequality follows from (3.7). Since k_1 is a fixed index, the above inequality implies that when k is sufficiently large, say $k \geqslant k'$, (3.14) holds. □

Lemma 3.6. *Under conditions* (1) *and* (2) *in Assumption* (A), *we have for an arbitrary* $v > 0$

$$\sum_{k=0}^{\infty} \|x_{k+1} - x^*\|^v < \infty \tag{3.15}$$

and

$$\sum_{k=0}^{\infty} \tau_k < \infty, \tag{3.16}$$

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

Proof. Denote $f_* = f(x^*)$. First, we show that there is a constant $a_3 > 0$ such that

$$f_{k+1} - f_* \leqslant (1 - a_3 \cos^2\phi_k)(f_k - f_*) \tag{3.17}$$

for all k sufficiently large. Indeed, (2.11) implies

$$f_{k+1} - f_* \leqslant (f_k - f_*) + \sigma_1 g_k^T s_k.$$

To show (3.17), it therefore suffices to verify that there is a constant $a_4 > 0$ such that when k is sufficiently large

$$g_k^{\mathrm{T}} s_k \leqslant -a_4 \cos^2 \phi_k (f_k - f_*). \tag{3.18}$$

Since x^* satisfies $g(x^*) = 0$, by Taylor's expansion, there is a constant $M_3 > 0$ such that $f_k - f_* \leqslant M_3 \|x_k - x^*\|^2$ for all k large enough. Thus from (3.11) and (3.13) we deduce that when k is sufficiently large

$$\begin{aligned} g_k^{\mathrm{T}} s_k &= -\|g_k\| \, \|s_k\| \cos \phi_k \\ &\leqslant -a_1' \|g_k\|^2 \cos^2 \phi_k \\ &\leqslant -a_1' m^2 \|x_k - x^*\|^2 \cos^2 \phi_k \\ &\leqslant -a_1' \frac{m^2}{M_3} \cos^2 \phi_k (f_k - f_*). \end{aligned}$$

Putting $a_4 = a_1' m_2^2 / M_3$ yields (3.18). Hence we get (3.17).

Now we prove (3.15). From Lemma 3.5 and the above discussion, we see that there exists an index $k_1' > 0$ such that when $k \geqslant k_1'$, (3.14) and (3.17) hold. Therefore

$$\begin{aligned} f_{k+1} - f_* &\leqslant (1 - a_3 \cos^2 \phi_k)(f_k - f_*) \\ &\quad \vdots \\ &\leqslant (f_{k_1'} - f_*) \prod_{i=k_1'}^{k} (1 - a_3 \cos^2 \phi_i) \\ &\leqslant (f_{k_1'} - f_*) \left[\frac{1}{k - k_1' + 1} \sum_{i=k_1'}^{k} (1 - a_3 \cos^2 \phi_i) \right]^{k - k_1' + 1} \\ &= (f_{k_1'} - f_*) \left[1 - a_3 \frac{1}{k - k_1' + 1} \sum_{i=k_1'}^{k} \cos^2 \phi_i \right]^{k - k_1' + 1} \\ &\leqslant (f_{k_1'} - f_*) \left[1 - a_3 \left(\prod_{i=k_1'}^{k} \cos^2 \phi_i \right)^{1/(k - k_1' + 1)} \right]^{k - k_1' + 1} \\ &= (f_{k_1'} - f_*) \left[1 - a_3 \left(\prod_{i=0}^{k} \cos^2 \phi_i \right)^{1/(k - k_1' + 1)} \left(\prod_{i=0}^{k_1' - 1} \cos^2 \phi_i \right)^{-1/(k - k_1' + 1)} \right]^{k - k_1' + 1} \\ &\leqslant (f_{k_1'} - f_*) \left[1 - a_3 a_2^{(k+1)/(k - k_1' + 1)} \left(\prod_{i=0}^{k_1' - 1} \cos^2 \phi_i \right)^{-1/(k - k_1' + 1)} \right]^{k - k_1' + 1}, \end{aligned}$$

where the last inequality follows from (3.14) in Lemma 3.5. Since k_1' is a constant, the second term in the last square bracket tends to a positive constant as k goes to infinity. Therefore, it follows that there is a constant $\rho_1 \in (0,1)$ such that when k is sufficiently large, $f_{k+1} - f_* \leqslant (f_{k_1'} - f_*)\rho_1^{k-k_1'+1}$. By Taylor's expansion and (3.12), we have $f_{k+1} - f_* \geqslant (m/2)\|x_{k+1} - x^*\|^2$ for all k sufficiently large. Therefore, we get

$$\begin{aligned}\|x_{k+1} - x^*\| &\leqslant \left[\frac{2}{m}(f_{k+1} - f_*)\right]^{1/2} \\ &= \sqrt{\rho_1}^{-k'+1}\left[\frac{2}{m}(f_{k'} - f_*)\right]^{1/2}\sqrt{\rho_1}^{k} \\ &\triangleq a_5\sqrt{\rho_1}^{k}.\end{aligned}$$

Hence we obtain (3.15) for an arbitrary $v > 0$.

Finally, since $\tau_k \leqslant \|x_k - x^*\|^v + \|x_{k+1} - x^*\|^v$, (3.16) follows from (3.15) directly. □

Lemma 3.7. *Let Assumption* (A) *hold. Denote* $Q = G(x^*)^{-1/2}$, $H_k = B_k^{-1}$, $H_{k+1} = B_{k+1}^{-1}$. *Then there are positive constants* b_i, $i = 1,2,\dots,7$ *and* $\alpha \in (0,1)$ *such that for all k sufficiently large*

$$\|B_{k+1} - G(x^*)\|_{Q,F} \leqslant (1 + b_1\tau_k)\|B_k - G(x^*)\|_{Q,F} + b_2\tau_k + b_3 r_k \tag{3.19}$$

and

$$\|H_{k+1} - G(x^*)^{-1}\|_{Q^{-1},F} \leqslant \left(\sqrt{1 - \alpha\mu_k^2} + b_4\tau_k + b_5 r_k\right)\|H_k - G(x^*)^{-1}\|_{Q^{-1},F} + b_6\tau_k + b_7 r_k, \tag{3.20}$$

where $\tau_k = \max\{\|x_k - x^*\|^v, \|x_{k+1} - x^*\|^v\}$, $\|A\|_{Q,F} = \|Q^{\mathrm{T}}AQ\|_F$, $\|\cdot\|_F$ *is the Frobenius norm of a matrix and*

$$\mu_k = \frac{\|Q^{-1}[H_k - G(x^*)^{-1}]y_k\|}{\|H_k - G(x^*)^{-1}\|_{Q^{-1},F}\|Qy_k\|}. \tag{3.21}$$

In particular, $\{\|B_k\|\}$ *and* $\{\|H_k\|\}$ *are bounded.*

Proof. From the update formula (2.12) we get

$$\begin{aligned}\|B_{k+1} - G(x^*)\|_{Q,F} &= \left\|B_k - G(x^*) - \frac{B_k s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k}\right\|_{Q,F} \\ &\leqslant \left\|B_k - G(x^*) - \frac{B_k s_k s_k^{\mathrm{T}} B_k}{s_k^{\mathrm{T}} B_k s_k} + \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}\right\|_{Q,F} + \left\|\frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k} - \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}\right\|_{Q,F} \\ &\leqslant (1 + b_1\tau_k)\|B_k - G(x^*)\|_{Q,F} + b_2\tau_k + \left\|\frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k} - \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}\right\|_{Q,F},\end{aligned} \tag{3.22}$$

where the last inequality follows from the inequality (49) in [10]. Moreover,

$$\begin{aligned}\left\|\frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}} s_k} - \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}\right\|_{Q,F} &= \left\|\frac{(\gamma_k + r_k s_k)(\gamma_k + r_k s_k)^{\mathrm{T}}}{(\gamma_k + r_k s_k)^{\mathrm{T}} s_k} - \frac{\gamma_k \gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}} s_k}\right\|_{Q,F} \\ &= \left\|\frac{\gamma_k^{\mathrm{T}} s_k(\gamma_k + r_k s_k)(\gamma_k + r_k s_k)^{\mathrm{T}} - (\gamma_k + r_k s_k)^{\mathrm{T}} s_k \gamma_k \gamma_k^{\mathrm{T}}}{(\gamma_k + r_k s_k)^{\mathrm{T}} s_k(\gamma_k^{\mathrm{T}} s_k)}\right\|_{Q,F} \\ &= r_k\left\|\frac{\gamma_k^{\mathrm{T}} s_k(\gamma_k s_k^{\mathrm{T}} + s_k \gamma_k^{\mathrm{T}} + r_k s_k s_k^{\mathrm{T}}) - \|s_k\|^2 \gamma_k \gamma_k^{\mathrm{T}}}{(\eta_k + r_k)\|s_k\|^2(\gamma_k^{\mathrm{T}} s_k)}\right\|_{Q,F}\end{aligned}$$

$$
\begin{aligned}
&\leqslant r_k\|Q\|_F^2\left\|\frac{\gamma_k^{\mathrm{T}}s_k(\gamma_k s_k^{\mathrm{T}}+s_k\gamma_k^{\mathrm{T}}+r_k s_k s_k^{\mathrm{T}})-\|s_k\|^2\gamma_k\gamma_k^{\mathrm{T}}}{(\eta_k+r_k)\|s_k\|^2(\gamma_k^{\mathrm{T}}s_k)}\right\|_F\\
&\leqslant r_k\|Q\|_F^2\,\frac{\gamma_k^{\mathrm{T}}s_k(\|\gamma_k s_k^{\mathrm{T}}\|_F+\|s_k\gamma_k^{\mathrm{T}}\|_F+r_k\|s_k s_k^{\mathrm{T}}\|_F)+\|s_k\|^2\|\gamma_k\gamma_k^{\mathrm{T}}\|_F}{(\eta_k+r_k)\|s_k\|^2(\gamma_k^{\mathrm{T}}s_k)}\\
&\leqslant r_k\,\frac{\|\gamma_k\|\,\|s_k\|(\|\gamma_k\|\,\|s_k\|+\|s_k\|\,\|\gamma_k\|+r_k\|s_k\|^2)+\|s_k\|^2\|\gamma_k\|^2}{(\eta_k+r_k)\|s_k\|^2(\gamma_k^{\mathrm{T}}s_k)}\,\|Q\|_F^2\\
&= r_k\,\frac{3\|\gamma_k\|^2+r_k\|\gamma_k\|\,\|s_k\|}{(\eta_k+r_k)(\gamma_k^{\mathrm{T}}s_k)}\,\|Q\|_F^2. \qquad (3.23)
\end{aligned}
$$

By the positive definiteness of $G(x^*)$, we see from (3.12) that when k is sufficiently large

$$\gamma_k^{\mathrm{T}}s_k=(g(x_{k+1})-g(x_k))^{\mathrm{T}}(x_{k+1}-x_k)\geqslant m\|x_{k+1}-x_k\|^2=m\|s_k\|^2.$$

Notice that $r_k\to 0$ by (3.10), $\eta_k+r_k\geqslant\varepsilon$ by (3.2), and $\|\gamma_k\|=\|g(x_{k+1})-g(x_k)\|\leqslant L\|s_k\|$ by (1.2). It then follows from (3.23) that there is a positive constant c_3 such that for all k sufficiently large

$$\left\|\frac{y_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}}s_k}-\frac{\gamma_k\gamma_k^{\mathrm{T}}}{\gamma_k^{\mathrm{T}}s_k}\right\|_{Q,F}\leqslant c_3 r_k.$$

Combining this and (3.22), we get (3.19).

Now we prove (3.20). We will use Lemma 3.1 in [4] to do this. First, it is well-known that the inverse update formula of (2.12) is given by

$$
\begin{aligned}
H_{k+1}&=H_k+\frac{(s_k-H_k y_k)s_k^{\mathrm{T}}+s_k(s_k-H_k y_k)^{\mathrm{T}}}{y_k^{\mathrm{T}}s_k}-\frac{y_k^{\mathrm{T}}(s_k-H_k y_k)s_k s_k^{\mathrm{T}}}{(y_k^{\mathrm{T}}s_k)^2}\\
&=\left(I-\frac{s_k y_k^{\mathrm{T}}}{y_k^{\mathrm{T}}s_k}\right)H_k\left(I-\frac{y_k s_k^{\mathrm{T}}}{y_k^{\mathrm{T}}s_k}\right)+\frac{s_k s_k^{\mathrm{T}}}{y_k^{\mathrm{T}}s_k}.
\end{aligned}
$$

This is the dual form of DFP update formula in the sense that $H_k\leftrightarrow B_k$, $H_{k+1}\leftrightarrow B_{k+1}$ and $s_k\leftrightarrow y_k$. We also have

$$
\begin{aligned}
\|Qy_k-Q^{-1}s_k\|&\leqslant\|Q\|\,\|y_k-Q^{-2}s_k\|\\
&=\|Q\|\,\|y_k-G(x^*)s_k\|\\
&=\|Q\|\,\|\gamma_k-G(x^*)s_k+r_k s_k\|\\
&\leqslant\|Q\|\left[\left\|\int_0^1 G(x_k+\tau s_k)s_k\,\mathrm{d}\tau-G(x^*)s_k\right\|+r_k\|s_k\|\right]\\
&\leqslant\|Q\|\left[\int_0^1\|G(x_k+\tau s_k)-G(x^*)\|\,\mathrm{d}\tau\|s_k\|+r_k\|s_k\|\right]\\
&\leqslant\|Q\|\left[M_2\int_0^1\|x_k-x^*+\tau s_k\|^{\nu}\,\mathrm{d}\tau+r_k\right]\|s_k\|\\
&\leqslant\|Q\|\left[M_2\int_0^1(\tau\|x_{k+1}-x^*\|+(1-\tau)\|x_k-x^*\|)^{\nu}\,\mathrm{d}\tau+r_k\right]\|s_k\|\\
&\leqslant\|Q\|(M_2\tau_k+r_k)\|s_k\|, \qquad (3.24)
\end{aligned}
$$

where M_2 is the Hölder constant for G in (3.9). Moreover, there exists a constant $b' > 0$ such that for all k large enough,

$$\begin{aligned}\|Qy_k\| &= \|Q(g(x_{k+1}) - g(x_k) + r_k s_k)\| \\ &\geqslant \|Q(g(x_{k+1}) - g(x_k))\| - r_k\|Qs_k\| \\ &\geqslant b'\|x_{k+1} - x_k\| - r_k\|Q\|\,\|s_k\| \\ &= (b' - r_k\|Q\|)\|s_k\|, \end{aligned} \tag{3.25}$$

where the second inequality follows from the positive definiteness of $G(x^*)$ and the fact that $x_k \to x^*$. Since $r_k \to 0$, (3.25) implies that there is a constant $c' > 0$ such that $\|Qy_k\| \geqslant c'\|s_k\|$ holds for all k sufficiently large. So, we get from (3.24)

$$\|Q^{-1}s_k - Qy_k\| \leqslant (c')^{-1}\|Q\|(M_2\tau_k + r_k)\|Qy_k\|. \tag{3.26}$$

Since $\tau_k \to 0$ by (3.16) and $r_k \to 0$ by (3.10), it is clear that when k is sufficiently large, $\|Qy_k - Q^{-1}s_k\| \leqslant \beta\|Qy_k\|$ for some constant $\beta \in (0, \frac{1}{3})$. Therefore, from Lemma 3.1 in [4] (with the identification $s \leftrightarrow y_k$, $y \leftrightarrow s_k$, $B \leftrightarrow H_k$, $\bar{B} \leftrightarrow H_{k+1}$, $A \leftrightarrow G(x^*)^{-1}$ and $M \leftrightarrow Q^{-1}$) (see also [1]), there are constants $\alpha \in (0, 1)$ and $b_4', b_5' > 0$ such that

$$\begin{aligned}\|H_{k+1} - G(x^*)^{-1}\|_{Q^{-1},F} \leqslant{} & \left(\sqrt{1 - \alpha\mu_k^2} + b_4'\frac{\|Q^{-1}s_k - Qy_k\|}{\|Qy_k\|}\right)\|H_k - G(x^*)\|_{Q^{-1},F} \\ & + b_5'\frac{\|s_k - G(x^*)^{-1}y_k\|}{\|Qy_k\|}, \end{aligned} \tag{3.27}$$

where μ_k is defined by (3.21). Since (3.26), we have

$$\begin{aligned}\frac{\|s_k - G(x^*)^{-1}y_k\|}{\|Qy_k\|} &= \frac{\|s_k - Q^2y_k\|}{\|Qy_k\|} \\ &= \frac{\|Q(Qy_k - Q^{-1}s_k)\|}{\|Qy_k\|} \\ &\leqslant \frac{\|Q\|\,\|Qy_k - Q^{-1}s_k\|}{\|Qy_k\|} \\ &\leqslant (c')^{-1}\|Q\|^2(M_2\tau_k + r_k). \end{aligned}$$

Combining this, (3.26) and (3.24) with (3.27), we get (3.20).

Finally, since $\sum_{k=0}^{\infty}\tau_k < \infty$ and $\sum_{k=0}^{\infty} r_k < \infty$, (3.19) and (3.20) together with Lemma 3.3 in [4] indicate that both $\|B_k - G(x^*)\|_{Q,F}$ and $\|H_k - G(x^*)^{-1}\|_{Q^{-1},F}$ converge. In particular, $\{\|B_k\|\}$ and $\{\|H_k\|\}$ are bounded. □

Now we establish superlinear convergence of MBFGS method.

Theorem 3.8. *Let Assumption* (A) *hold. If the parameter* σ_1 in (2.11) *is chosen to satisfy* $\sigma_1 \in (0, \frac{1}{2})$, *then* $\{x_k\}$ *converges to* x^* *superlinearly.*

Proof. We first show that the Dennis–Moré condition

$$\lim_{k\to\infty}\frac{\|(B_k - G(x^*))s_k\|}{\|s_k\|} = 0 \tag{3.28}$$

holds. Since $\sqrt{1-t} \leqslant 1-\frac{1}{2}t$, $\forall t \in (0,1)$, $\|s_k\| \to 0$, $\tau_k \to 0$ and $\{\|H_k\|\}$ is bounded, it follows from (3.20) that there are positive constants M_4 and M_5 such that for all k sufficiently large

$$\|H_{k+1} - G(x^*)^{-1}\|_{Q^{-1},F} \leqslant (1 - \tfrac{1}{2}\alpha\mu_k^2)\|H_k - G(x^*)^{-1}\|_{Q^{-1},F} + M_4\tau_k + M_5 r_k,$$

i.e.,

$$\tfrac{1}{2}\alpha\mu_k^2\|H_k - G(x^*)^{-1}\|_{Q^{-1},F} \leqslant \|H_k - G(x^*)^{-1}\|_{Q^{-1},F} - \|H_{k+1} - G(x^*)^{-1}\|_{Q^{-1},F} + M_4\tau_k + M_5 r_k.$$

Summing these inequalities we get

$$\frac{1}{2}\alpha \sum_{k=\tilde{k}}^{\infty} \mu_k^2 \|H_k - G(x^*)^{-1}\|_{Q^{-1},F} < \infty,$$

where $\tilde{k}$ is a sufficiently large index such that (3.20) holds for all $k \geqslant \tilde{k}$. In particular, we have $\lim_{k\to\infty} \mu_k^2 \|H_k - G(x^*)^{-1}\|_{Q^{-1},F} = 0$, i.e.,

$$\lim_{k\to\infty} \frac{\|Q^{-1}(H_k - G(x^*)^{-1})y_k\|^2}{\|H_k - G(x^*)^{-1}\|_{Q^{-1},F}\|Qy_k\|^2} = 0.$$

However, since $\{\|H_k - G(x^*)^{-1}\|_{Q^{-1},F}\}$ is bounded, this inequality implies that

$$\lim_{k\to\infty} \frac{\|Q^{-1}(H_k - G(x^*)^{-1})y_k\|}{\|Qy_k\|} = 0. \tag{3.29}$$

Moreover we have

$$\begin{aligned}
\|Q^{-1}(H_k - G(x^*)^{-1})y_k\| &= \|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}y_k\| \\
&\geqslant \|Q^{-1}H_k(G(x^*) - B_k)s_k\| - \|Q^{-1}H_k(G(x^*) - B_k)(s_k - G(x^*)^{-1}y_k)\| \\
&\geqslant \|Q^{-1}H_k(G(x^*) - B_k)s_k\| - \|Q^{-1}H_k(G(x^*) - B_k)(s_k - G(x^*)^{-1}\gamma_k)\| \\
&\quad - r_k\|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}s_k\|.
\end{aligned} \tag{3.30}$$

Note that

$$\begin{aligned}
&\|Q^{-1}H_k(G(x^*) - B_k)(s_k - G(x^*)^{-1}\gamma_k)\| \\
&\quad = \|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}(G(x^*)s_k - \gamma_k)\| \\
&\quad = \|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}[(G(x^*) - G(x_k))s_k + (G(x_k)s_k - \gamma_k)]\| \\
&\quad \leqslant \|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}\|\{\|G(x^*) - G(x_k)\|\,\|s_k\| + \|G(x_k)s_k - \gamma_k\|\} \\
&\quad = o(\|s_k\|)
\end{aligned}$$

and

$$r_k\|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}s_k\| \leqslant r_k\|Q^{-1}H_k(G(x^*) - B_k)G(x^*)^{-1}\|\,\|s_k\| = o(\|s_k\|),$$

where we used the fact that $\{\|B_k\|\}$ and $\{\|H_k\|\}$ are bounded (and hence uniformly nonsingular), G is continuous and $r_k \to 0$. Therefore, it follows from (3.30) that for some constant $m_1 > 0$

$$\|Q^{-1}(H_k - G(x^*)^{-1})y_k\| \geqslant m_1\|(G(x^*) - B_k)s_k\| - o(\|s_k\|). \tag{3.31}$$

On the other hand, we have from (3.5) in Lemma 3.1

$$\|Qy_k\| \leqslant \|Q\|\,\|y_k\| \leqslant (L + r)\|Q\|\,\|s_k\|. \tag{3.32}$$

From (3.31), (3.32) and (3.29), we conclude that the Dennis–Moré condition (3.28) holds.

Next we verify that $\lambda \equiv 1$ for all k sufficiently large. Since $\|p_k\| = \|H_k g_k\| \to 0$, by Taylor's expansion we obtain

$$\begin{aligned} f(x_k + p_k) - f(x_k) - \sigma_1 g(x_k)^{\mathrm{T}} p_k &= (1-\sigma_1) g(x_k)^{\mathrm{T}} p_k + \tfrac{1}{2} p_k^{\mathrm{T}} G(x_k + \bar{\theta}_k p_k) p_k \\ &= -(1-\sigma_1) p_k^{\mathrm{T}} B_k p_k + \tfrac{1}{2} p_k^{\mathrm{T}} G(x_k + \bar{\theta}_k p_k) p_k \\ &= -(\tfrac{1}{2} - \sigma_1) p_k^{\mathrm{T}} B_k p_k - \tfrac{1}{2} p_k^{\mathrm{T}} (B_k - G(x_k + \bar{\theta}_k p_k)) p_k \\ &= -(\tfrac{1}{2} - \sigma_1) p_k^{\mathrm{T}} G(x^*) p_k + \mathrm{o}(\|p_k\|^2), \end{aligned}$$

where $\bar{\theta}_k \in (0,1)$ and the last equality follows from (3.28). Thus $f(x_k + p_k) - f(x_k) - \sigma_1 g(x_k)^{\mathrm{T}} p_k \leqslant 0$ for all k sufficiently large. In other words, $\lambda_k = 1$ satisfies the first inequality of (2.11) for all k sufficiently large.

On the other hand, we have

$$\begin{aligned} g(x_k + p_k)^{\mathrm{T}} p_k - \sigma_2 g(x_k)^{\mathrm{T}} p_k &= (g(x_k + p_k) - g(x_k))^{\mathrm{T}} p_k + (1-\sigma_2) g(x_k)^{\mathrm{T}} p_k \\ &= p_k^{\mathrm{T}} G(x_k + \bar{\theta}'_k p_k) p_k - (1-\sigma_2) p_k^{\mathrm{T}} B_k p_k \\ &= p_k^{\mathrm{T}} G(x_k + \bar{\theta}'_k p_k) p_k - (1-\sigma_2) p_k^{\mathrm{T}} G(x_k) p_k + \mathrm{o}(\|p_k\|^2) \\ &= \sigma_2 p_k^{\mathrm{T}} G(x_k) p_k + \mathrm{o}(\|p_k\|^2), \end{aligned}$$

where $\bar{\theta}'_k \in (0,1)$. So we have $g(x_k + p_k)^{\mathrm{T}} p_k \geqslant \sigma_2 g_k^{\mathrm{T}} p_k$, which means that $\lambda_k = 1$ satisfies the second inequality of (2.11) for all k sufficiently large. Therefore, we assert that the unit stepsize is accepted when k is sufficiently large. Consequently, we can deduce that $\{x_k\}$ converges superlinearly. □

4. A practicable MBFGS method

In Section 3, we have proposed a general modification of BFGS method. We have also shown that if r_k is chosen to satisfy (3.2) then under appropriate conditions, the modified BFGS method converges globally. If in addition (3.10) holds, then the convergence rate is superlinear. In other words, the global and superlinear convergence of MBFGS method depends on the choice of $\{r_k\}$. Therefore, it is important to select $\{r_k\}$ appropriately so that it is practicable and satisfies (3.2) and (3.10). The following theorem shows that $r_k = \mathrm{O}(\|g_k\|)$ is a suitable choice.

Theorem 4.1. *Suppose that the level set Ω is bounded. Let $\{x_k\}$ be generated by MBFGS method with B_k being updated by* (2.12). *If the parameters r_k are chosen as $r_k = \vartheta_k \|g_k\|$, where $\underline{\vartheta} \leqslant \vartheta_k \leqslant \bar{\vartheta}$ for all k with some constants $0 < \underline{\vartheta} < \bar{\vartheta}$, then we have*

$$\liminf_{k \to \infty} \|g_k\| = 0. \tag{4.1}$$

If in addition, conditions (1)–(3) *in Assumption* (A) *hold and the parameter σ_1 in* (2.11) *is chosen to satisfy $\sigma_1 \in (0, \frac{1}{2})$, then $\{x_k\}$ converges superlinearly.*

Proof. Denote by $\bar{M}$ an upper bound of $\{\|g_k\|\}$ on Ω. It is obvious that $r_k \leqslant \bar{\vartheta}\bar{M}$. This means that r_k varies in a bounded interval $[0, \bar{\vartheta}\bar{M}]$.

To prove (4.1), we assume to the contrary that $\|g_k\| \geqslant \gamma$ holds for all k with some constant $\gamma > 0$. Then we have

$$\eta_k + r_k = \frac{\gamma_k^{\mathrm{T}} s_k}{\|s_k\|^2} + \vartheta_k \|g_k\| \geqslant -\frac{(1-\sigma_2) g_k^{\mathrm{T}} s_k}{\|s_k\|^2} + \underline{\vartheta}\gamma \geqslant \underline{\vartheta}\gamma,$$

where the first inequality follows from (2.11). This shows that inequality (3.2) holds with $\varepsilon = \underline{\vartheta}\gamma$. Therefore, by Theorem 3.1 we get a contradiction.

If in addition, conditions (1)–(3) in Assumption (A) hold, then we get from (3.12) that $\gamma_k^{\mathrm{T}} s_k = s_k^{\mathrm{T}} \int_0^1 G(x_k + \tau s_k)\,\mathrm{d}\tau\, s_k \geqslant m\|s_k\|^2$ for all k large enough. Thus

$$\eta_k + r_k = \frac{\gamma_k^{\mathrm{T}} s_k}{\|s_k\|^2} + \vartheta_k \|g_k\| \geqslant \frac{\gamma_k^{\mathrm{T}} s_k}{\|s_k\|^2} \geqslant m.$$

This shows that (3.2) holds for all k sufficiently large with $\varepsilon = m$.

Moreover, Lemma 3.6 indicates that conditions (1) and (2) in Assumption (A) imply $\sum_{k=0}^{\infty} \|x_k - x^*\| < \infty$. Since

$$r_k = \vartheta_k \|g_k\| = \vartheta_k \|g(x_k) - g(x^*)\| \leqslant \bar{\vartheta} L \|x_k - x^*\|,$$

it follows that $\{r_k\}$ satisfies (3.10), i.e., condition (4) in Assumption (A) is fulfilled. Therefore, from Theorem 3.8 we get the superlinear convergence of $\{x_k\}$. This completes the proof. □

5. Backtracking line search

In this section, we extend the results obtained in the previous sections to MBFGS method with backtracking line search. Specifically, we consider the algorithm in which line search condition (2.11) is replaced by the following inequality:

$$f(x_k + \lambda_k p_k) \leqslant f(x_k) + \sigma \lambda_k g_k^{\mathrm{T}} p_k, \tag{5.1}$$

where $\sigma \in (0,1)$ is a given constant and λ_k is the largest element in the set $\{1, \rho, \rho^2, \ldots\}$ with $\rho \in (0,1)$ which satisfies (5.1).

However, in this case, the condition $y_k^{\mathrm{T}} s_k > 0$ may fail to be fulfilled and the hereditary positive definiteness of B_k is not guaranteed any more. To cope with this defect, we further modify the vector y_k as $y_k = \gamma_k + t_k \|g_k\| s_k$, where $t_k > 0$ is determined by

$$t_k = 1 + \max\left\{ -\frac{\gamma_k^{\mathrm{T}} s_k}{\|s_k\|^2}, 0 \right\}. \tag{5.2}$$

Then it is easy to see that we always have $y_k^{\mathrm{T}} s_k \geqslant \|g_k\|\,\|s_k\|^2$.

With this modification, we present the following algorithm.

Algorithm 2 (Modified BFGS method with backtracking line search)**.**

Step 0: Choose an initial point $x_0 \in \mathbb{R}^n$, an initial positive definite matrix B_0, and constants $\sigma \in (0,1)$ and $\rho \in (0,1)$. Let $k := 0$.

Step 1: Solve the following linear equation to get p_k:

$$B_k p + g_k = 0. \tag{5.3}$$

Step 2: Find the smallest nonnegative integer j, say j_k, satisfying

$$f(x_k + \rho^j p_k) \leqslant f(x_k) + \sigma \rho^j g_k^T p_k \tag{5.4}$$

and let $\lambda_k = \rho^{j_k}$.

Step 3: Let the next iterate be $x_{k+1} = x_k + \lambda_k p_k$.

Step 4: Update B_k using the formula

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}, \tag{5.5}$$

where $s_k = x_{k+1} - x_k = \lambda_k p_k$ and $y_k = \gamma_k + t_k \|g_k\| s_k$ with t_k given by (5.2).

Step 5: Let $k := k + 1$ and go to Step 1.

We note that the difference between Algorithms 1 and 2 lies in the line search (Step 2) and the expression of y_k.

Lemma 5.1. *Suppose that the level set Ω is bounded. Let $\{x_k\}$ be generated by Algorithm* 2. *If $\|g_k\| \geqslant \zeta$ holds for all k with some constant $\zeta > 0$, then there are positive constants β_j, $j = 1,2,3$ such that, for any k, the inequalities*

$$\|B_i s_i\| \leqslant \beta_1 \|s_i\| \quad \text{and} \quad \beta_2 \|s_i\|^2 \leqslant s_i^T B_i s_i \leqslant \beta_3 \|s_i\|^2 \tag{5.6}$$

hold for at least a half of the indices $i \in \{1,2,\dots,k\}$.

Proof. It is easy to see that $\{x_k\} \subset \Omega$ and $\|y_k\| \leqslant C\|s_k\|$ for some positive constant C. By the choice of t_k, we have $y_k^T s_k \geqslant \|g_k\| \, \|s_k\|^2 \geqslant \zeta \|s_k\|^2$. Therefore, the proof follows from that of Theorem 2.1 in [2]. □

Lemma 5.2. *Let the level set Ω be bounded. If $\|g_k\| \geqslant \zeta$ holds for all k with some constant $\zeta > 0$, then there is a positive constant $\bar{\lambda}$ such that $\lambda_i \geqslant \bar{\lambda}$ for all $i \in J = \{i \,|\, (5.6) \text{ holds}\}$.*

Proof. It suffices to consider the case $\lambda_i \neq 1$. By the line search rule, we see that $\lambda_i' \equiv \lambda_i/\rho$ does not satisfy inequality (5.1), i.e.,

$$f(x_i + \lambda_i' p_i) - f(x_i) > \sigma \lambda_i' g_i^T p_i. \tag{5.7}$$

By the mean-value theorem and (1.2) we have

$$\begin{aligned} f(x_i + \lambda_i' p_i) &= f(x_i) + \lambda_i' g(x_i)^T p_i + \lambda_i' (g(x_i + \theta_i \lambda_i' p_i) - g(x_i))^T p_i \\ &\leqslant f(x_i) + \lambda_i' g(x_i)^T p_i + (\lambda_i')^2 L \|p_i\|^2, \end{aligned}$$

where $\theta_i \in (0,1)$. Substituting this into (5.7), we get for all $i \in J$,

$$\begin{aligned} \lambda_i' L \|p_i\|^2 &> -(1-\sigma) g(x_i)^T p_i \\ &= (1-\sigma) p_i^T B_i p_i \\ &\geqslant (1-\sigma)\beta_2 \|p_i\|^2, \end{aligned}$$

where the last inequality follows from (5.6). This means that $\lambda_i' \geqslant ((1-\sigma)/L)\beta_2$ and hence $\lambda_i = \lambda_i' \rho \geqslant (1-\sigma)\beta_2 \rho / L \triangleq \bar{\lambda} > 0$ for all $i \in J$. □

A global convergence theorem for Algorithm 2 is now stated as follows.

Theorem 5.1. *Let the level set* Ω *be bounded and* $\{x_k\}$ *be generated by Algorithm* 2. *Then we have*

$$\liminf_{k\to\infty} \|g_k\| = 0.$$

Proof. Suppose to the contrary that $\|g_k\| \geqslant \zeta$ holds for all k with some $\zeta > 0$. Summing (5.1) we have

$$\begin{aligned}
\infty &> \sum_{k=0}^{\infty}(-g_k^{\mathrm{T}}s_k) \\
&= \sum_{k=0}^{\infty} \|g_k\|^2 \lambda_k \frac{s_k^{\mathrm{T}}B_k s_k}{\|B_k s_k\|^2} \\
&\geqslant \zeta^2 \sum_{k=0}^{\infty} \lambda_k \frac{s_k^{\mathrm{T}}B_k s_k}{\|B_k s_k\|^2} \\
&\geqslant \zeta^2 \sum_{k\in J} \lambda_k \frac{s_k^{\mathrm{T}}B_k s_k}{\|B_k s_k\|^2} \\
&\geqslant \zeta^2 \bar{\lambda} \sum_{k\in J} \frac{s_k^{\mathrm{T}}B_k s_k}{\|B_k s_k\|^2}.
\end{aligned}$$

Then, in a similar manner to the proof of Theorem 3.4, we can prove the theorem. □

It is easy to see that if conditions (1) and (2) in Assumption (A) hold, then $t_k \equiv 1$ holds for all k sufficiently large. Therefore, we can establish superlinear convergence of Algorithm 2 in a similar manner to Theorem 3.2.

Theorem 5.2. *Let conditions* (1)–(3) *in Assumption* (A) *hold. If the parameter* σ *in* (5.4) *is chosen to satisfy* $\sigma \in (0, \frac{1}{2})$, *then the sequence* $\{x_k\}$ *generated by Algorithm* 2 *converges to* x^* *superlinearly.*

Proof. Omitted. □

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