A modified scaling BFGS method for nonconvex minimization

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Abstract In this paper, we propose a modified scaling BFGS method for unconstrained minimization. A remarkable feature of the proposed method is that it can improve the performance of the BFGS method and possesses a global convergence property without convexity assumption on the objective function. Under certain assumptions, we also establish superlinear convergence of the method. Finally we show numerical results.

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§1. Introduction

This paper is concerned with the unconstrained minimization problem

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

where $f: \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable. In the following, g(x) and G(x) denote the gradient and Hessian matrix of f at x, respectively. Quasi-Newton methods are effective numerical methods for solving (1.1), and they are iterative methods of the form

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

where x_k is a current approximation to a solution for (1.1), α_k is a step size and d_k is a search direction obtained by solving the linear system of equations

$$B_k d_k = -g_k$$
.

Here g_k denotes $g(x_k)$ and the matrix B_k is an approximation to $G_k \equiv G(x_k)$. The matrix B_k is updated at every iteration by means of a quasi-Newton updating formula. There are some kinds of updating formulas. In particular, the BFGS formula is one of the most effective formulas and is given by

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

where

$$s_k = x_{k+1} - x_k$$
 and $y_k = g_{k+1} - g_k$.

Throughout this paper, let f_k denote $f(x_k)$.

The BFGS method is widely used due to its favorable numerical experience and fast convergence property. However, the performance of the conventional BFGS method may be greatly influenced by an unsuitable search direction when the Hessian matrix is ill-conditioned. To overcome this difficulty, several researchers proposed scaling BFGS methods. For example, Oren and Luenberger [14, 13] suggested a class of the method that they referred to as self-scaling variable metric methods (SSVMs). They multiplied B_k by an appropriate scalar ω_k before it was updated, and they used the sized BFGS updating formula

$$B_{k+1} = \omega_k \left(B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} \right) + \frac{y_k y_k^T}{y_k^T s_k},$$

in which the parameter ω_k was chosen as

$$\omega_k^{OL} = \frac{y_k^T s_k}{s_k^T B_k s_k}, \qquad \omega_k^{IOL} = \frac{y_k^T B_k^{-1} y_k}{y_k^T s_k},$$

which can accelerate the single-step convergence of quasi-Newton methods for a quadratic objective function. Another choice of ω_k is given by Al-Baali [2] as follows

$$\omega_k^{AB} = \min \left\{ \frac{y_k^T s_k}{s_k^T B_k s_k}, 1 \right\}.$$

In [2], Al-Baali showed that the sized BFGS method with ω_k^{AB} is competitive with the standard BFGS method. Furthermore, other choices of ω_k and numerical results were derived by Al-Baali [1, 2], Nocedal and Yuan [11] and Yabe et al. [16], for example.

More recently, a different scaling BFGS method was derived by Cheng and Li [5]. In order to improve the condition number of the Hessian matrix, they noticed the following approximate relation

(1.2)
$$\gamma_k f(x)$$

$$\approx \gamma_k \left(f_{k+1} + g_{k+1}^T (x - x_{k+1}) + \frac{1}{2} (x - x_{k+1})^T G_{k+1} (x - x_{k+1}) \right),$$

where γ_k is some scalar. Differentiating (1.2) and substituting x_k into x yield the relation

$$\gamma_k G_{k+1} s_k \approx \gamma_k y_k$$

from which they proposed a new secant condition:

$$(1.3) B_{k+1}s_k = \gamma_k y_k.$$

We call γ_k the scaling factor in this paper. In [5], they chose the following scaling factor

(1.4)
$$\gamma_k^{CL} = \frac{y_k^T s_k}{\|y_k\|^2}.$$

Based on (1.3) and (1.4), B_k is updated by

(1.5)
$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \gamma_k^{CL} \frac{y_k y_k^T}{y_k^T s_k}.$$

They called the method based on (1.4) and (1.5) the spectral scaling BFGS method. By using this method, the largest eigenvalue of B_k is strictly less than $\text{Tr}(B_1)+k$. Therefore, the spectral scaling BFGS method has a good self-correcting property with respect to the trace of B_k . Moreover, they showed the global convergence of their method for a uniformly convex objective function and good numerical performance in [5]. Yuan [17] also proposed a modified BFGS method.

Besides, several researchers studied another secant condition:

$$(1.6) B_{k+1}s_k = \hat{y}_k, \hat{y}_k = y_k + \phi_k s_k.$$

Li and Fukushima [9] showed that under some conditions the modified BFGS method based on (1.6) with a nonnegative parameter ϕ_k has a global convergence property without convexity assumption on the objective function. In addition, they also established superlinear convergence of their method.

In this paper, we study a scaling BFGS method with $\gamma_k \hat{y}_k$ (We call the modified scaling BFGS method) and obtain the global convergence property without convexity assumption of f. Moreover, we also establish the superlinear convergence of the method. In addition, we apply a new scaling factor to the

method and prove its convergence property.

We organize the paper as follows. In the next section, we propose a modified scaling BFGS method. In Section 3, we prove the global and superlinear convergence of our method. In Section 4, we apply new scaling factors to the method and establish its convergence property. Finally, in Section 5, we present some numerical experiments.

§2. Modified scaling BFGS method

In this section, we propose a modified scaling BFGS method. First, we recall the modification to the standard BFGS method in [9]. Note that if f is twice continuously differentiable, we have the following approximation

$$(2.1) G_{k+1}s_k \approx y_k,$$

which yields the secant condition $B_{k+1}s_k = y_k$. So the approximate matrix of G_{k+1} is usually produced based on (2.1). However, since G_{k+1} is not generally positive definite when f is nonconvex, B_{k+1} may not afford a good approximation of G_{k+1} . To overcome this difficulty, we can replace G_{k+1} by the matrix

$$\bar{G}_{k+1} \equiv G_{k+1} + \phi_k I$$
,

where I is the identity matrix and ϕ_k is chosen so that \bar{G}_{k+1} is positive definite. The matrix \bar{G}_{k+1} will satisfy the following relation

(2.2)
$$\bar{G}_{k+1}s_k = (G_{k+1} + \phi_k I)s_k \approx \hat{y}_k,$$

where \hat{y}_k is defined by (1.6). Li and Fukushima [9] used the modified secant condition (1.6) based on (2.2).

Following the idea of Cheng and Li [5], we multiply the both sides of (2.2) by a scaling factor γ_k as follows

$$\gamma_k \bar{G}_{k+1} s_k \approx \gamma_k \hat{y}_k$$
.

This leads to the following secant condition

$$(2.3) B_{k+1}s_k = \gamma_k \hat{y}_k.$$

When $\gamma_k = 1$ and $\phi_k = 0$, we get the standard secant condition. An appropriate choice of γ_k and ϕ_k may give a scaling BFGS method which has a global convergence property without convexity assumption of f and good numerical results. In Section 4, we will present several concrete choices of γ_k and ϕ_k .

Now, we propose the modified scaling BFGS method (msBFGS) based on (2.3).

[Algorithm of the msBFGS method]

Step 0. Choose an initial point $x_0 \in R^n$ and an initial symmetric positive definite matrix $B_0 \in R^{n \times n}$. 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 system of equations to obtain d_k :

$$B_k d_k = -g_k$$
.

Step 2. Find a step size α_k satisfying the Wolfe conditions:

$$(2.4) f(x_k + \alpha_k d_k) \le f(x_k) + \sigma_1 \alpha_k g_k^T d_k,$$

$$(2.5) g(x_k + \alpha_k d_k)^T d_k \ge \sigma_2 g_k^T d_k.$$

Step 3. Let the next iterate be $x_{k+1} = x_k + \alpha_k d_k$.

Step 4. If the stopping condition is satisfied, then stop. Otherwise go to Step 5

Step 5. Give $\gamma_k > 0$ and $\phi_k \in [0, C]$. Let $\hat{y}_k = y_k + \phi_k s_k$.

Step 6. Update B_k by using the msBFGS formula

(2.6)
$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \gamma_k \frac{\hat{y}_k \hat{y}_k^T}{\hat{y}_k^T s_k}.$$

Step 7. Let k := k + 1 and go to Step 1.

It follows from $\gamma_k > 0$, $\phi_k \ge 0$ and (2.5) that for any k

(2.7)
$$\gamma_k \hat{y}_k^T s_k \ge \gamma_k y_k^T s_k > 0.$$

Therefore, the matrix B_{k+1} is positive definite as long as B_k is positive definite. Consequently, d_k becomes a descent search direction of f at x_k .

§3. Convergence analysis

In this section, we will establish the global and superlinear convergence property of the msBFGS method. To this end, we make the following assumptions.

Assumption A

(1) The level set at the initial point x_0

$$\Omega = \{ x \in \mathbb{R}^n \mid f(x) \le f(x_0) \}$$

is bounded.

(2) The objective function f is continuously differentiable in an open convex set containing Ω , and there exists a positive constant L_g such that

$$||g(x) - g(y)|| \le L_q ||x - y||$$
 for all $x, y \in \Omega$.

Now we analyze convergence properties of our method. The global convergence is proved in Section 3.1, and the local and superlinear convergence is shown in Section 3.2.

In the remainder of this paper, let

(3.1)
$$\cos \theta_k = \frac{s_k^T B_k s_k}{\|s_k\| \|B_k s_k\|},$$

(3.2)
$$q_k = \frac{s_k^T B_k s_k}{\|s_k\|^2},$$

$$\Psi(B_k) = \operatorname{Tr}(B_k) - \ln(\det B_k)$$

and

$$(3.3) z_k = \gamma_k \hat{y}_k.$$

Note that $\Psi(B_k)$ can be represented by the expression

(3.4)
$$\Psi(B_k) = \sum_{j=1}^{n} (\mu_{k,j} - \ln \mu_{k,j}),$$

where $0 < \mu_{k,1} \le \cdots \le \mu_{k,n}$ are the eigenvalues of B_k . We also note that the function

$$w(p) = p - \ln(p), \qquad p > 0$$

is strictly convex and has the minimum value of 1 at p=1. Therefore, $\Psi(B_k) \geq n$ holds. Taking the trace in the msBFGS formula, we get

$$\operatorname{Tr}(B_{k+1}) = \operatorname{Tr}(B_k) - \frac{\|B_k s_k\|^2}{s_k^T B_k s_k} + \frac{\|z_k\|^2}{z_k^T s_k}.$$

Furthermore, taking the determinant in the msBFGS formula, we have

$$\det(B_{k+1}) = \det\left(B_k \left(I - \frac{s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{B_k^{-1} z_k z_k^T}{z_k^T s_k}\right)\right)
= \det(B_k) \left(1 - \frac{s_k^T}{s_k^T B_k s_k} B_k s_k\right) \left(1 + \frac{(B_k^{-1} z_k)^T}{z_k^T s_k} z_k\right)
- \det(B_k) \left(\frac{-z_k^T s_k}{s_k^T B_k s_k}\right) \left(\frac{s_k^T B_k B_k^{-1} z_k}{z_k^T s_k}\right)
= \det(B_k) \frac{z_k^T s_k}{s_k^T B_k s_k},$$

where the second equality can be found in Lemma 7.6 of [7]. Therefore, we derive the following expression for $\Psi(B_k)$.

$$\begin{split} &\Psi(B_{k+1}) \\ &= \Psi(B_k) - \frac{\|B_k s_k\|^2}{s_k^T B_k s_k} + \frac{\|z_k\|^2}{z_k^T s_k} - \ln\left(\frac{z_k^T s_k}{s_k^T B_k s_k}\right) \\ &= \Psi(B_k) - \left(\frac{\|B_k s_k\| \|s_k\|}{s_k^T B_k s_k}\right)^2 \frac{s_k^T B_k s_k}{\|s_k\|^2} + \frac{\|z_k\|^2}{z_k^T s_k} - \ln\left(\frac{z_k^T s_k}{\|s_k\|^2} \frac{\|s_k\|^2}{s_k^T B_k s_k}\right). \end{split}$$

Using the definitions (3.1) and (3.2), we have

$$(3.5) \qquad \Psi(B_{k+1}) = \Psi(B_k) + \frac{\|z_k\|^2}{z_k^T s_k} - \ln \frac{z_k^T s_k}{\|s_k\|^2} - \frac{q_k}{\cos^2 \theta_k} + \ln q_k$$

$$= \Psi(B_k) + \frac{\|z_k\|^2}{z_k^T s_k} - \ln \frac{z_k^T s_k}{\|s_k\|^2} + \ln \cos^2 \theta_k - 1$$

$$+ \left(1 - \frac{q_k}{\cos^2 \theta_k} + \ln \frac{q_k}{\cos^2 \theta_k}\right).$$

3.1. Global convergence

To prove the global convergence, we first introduce the following general result (see Theorem 3.2 of [12]).

Lemma 3.1. Suppose that Assumption A holds. Consider any iterative method of the form $x_{k+1} = x_k + \alpha_k d_k$, where a search direction d_k satisfies the descent condition $g_k^T d_k < 0$ and a step size α_k satisfies the Wolfe conditions (2.4) and

(2.5). Then the following Zoutendijk condition holds

(3.6)
$$\sum_{k=0}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty.$$

The next lemma gives the conditions on γ_k and ϕ_k and is useful in showing the global convergence.

Lemma 3.2. Let B_0 be symmetric positive definite and B_k be updated by (2.6). Suppose that there exist positive constants m, M and t_1 such that for any $k \geq t_1$, γ_k and ϕ_k satisfy

$$(3.7) \gamma_k(\rho_k^{(1)} + \phi_k) \geq m,$$

(3.8)
$$\gamma_k(\rho_k^{(2)} + 2\phi_k\rho_k^{(1)} + \phi_k^2) \leq M(\rho_k^{(1)} + \phi_k),$$

where $\rho_k^{(1)} = \frac{y_k^T s_k}{\|s_k\|^2}$ and $\rho_k^{(2)} = \frac{\|y_k\|^2}{\|s_k\|^2}$. Then there exist positive constants β_0 , β_1 , β_2 and β_3 such that for any positive integer $k \ (\geq t_1)$, the following inequalities

$$(3.9) \cos \theta_j \geq \beta_0,$$

(3.11)
$$\beta_2 \|s_j\|^2 \le s_j^T B_j s_j \le \beta_3 \|s_j\|^2$$

hold at least $\lceil (k-t_1+1)/2 \rceil$ values of $j \in \{t_1, \ldots, k\}$.

Proof. We can prove this lemma similarly to the proof of Theorem 2.1 in [4]. We first note that

(3.12)
$$\rho_k^{(1)} + \phi_k = \frac{\hat{y}_k^T s_k}{\|s_k\|^2}$$

and

$$(3.13) \frac{\rho_k^{(2)} + 2\phi_k \rho_k^{(1)} + \phi_k^2}{\rho_k^{(1)} + \phi_k} = \frac{\|y_k\|^2 + 2\phi_k y_k^T s_k + \phi_k^2 \|s_k\|^2}{y_k^T s_k + \phi_k \|s_k\|^2} = \frac{\|\hat{y}_k\|^2}{\hat{y}_k^T s_k}.$$

From (3.3), (3.7), (3.8), (3.12) and (3.13), we have

$$\frac{z_k^T s_k}{\|s_k\|^2} = \gamma_k \frac{\hat{y}_k^T s_k}{\|s_k\|^2} = \gamma_k (\rho_k^{(1)} + \phi_k) \ge m$$

and

$$\frac{\|z_k\|^2}{z_k^T s_k} = \gamma_k \frac{\|\hat{y}_k\|^2}{s_k^T \hat{y}_k} = \gamma_k \frac{\rho_k^{(2)} + 2\phi_k \rho_k^{(1)} + \phi_k^2}{\rho_k^{(1)} + \phi_k} \le M.$$

Thus, it follows from (3.5) that

$$\Psi(B_{k+1}) \leq \Psi(B_k) + M - \ln m + \ln \cos^2 \theta_k - 1 + \left(1 - \frac{q_k}{\cos^2 \theta_k} + \ln \frac{q_k}{\cos^2 \theta_k}\right) \\
\leq \dots \\
\leq \Psi(B_{t_1}) + (M - \ln m - 1)(k - t_1 + 1) \\
+ \sum_{j=t_1}^k \left(\ln \cos^2 \theta_j + \left(1 - \frac{q_j}{\cos^2 \theta_j} + \ln \frac{q_j}{\cos^2 \theta_j}\right)\right).$$

Let us define η_i by

(3.14)
$$\eta_j = -\ln\cos^2\theta_j - \left(1 - \frac{q_j}{\cos^2\theta_j} + \ln\frac{q_j}{\cos^2\theta_j}\right).$$

The function

$$(3.15) u(p) = 1 - p + \ln p$$

achieves the maximum value of 0 at p = 1. Thus, $\eta_j \ge 0$ holds. Furthermore, since $\Psi(B_{k+1}) > 0$, we have

(3.16)
$$\frac{1}{k-t_1+1} \sum_{j=t_1}^k \eta_j < \frac{\Psi(B_{t_1})}{k-t_1+1} + (M-1-\ln m).$$

Let us now define J_k to be a set consisting of the $\left\lceil \frac{k-t_1+1}{2} \right\rceil$ indices corresponding to the $\left\lceil \frac{k-t_1+1}{2} \right\rceil$ smallest values of η_j for $t_1 \leq j \leq k$, and let η_{mk} denote the largest value of η_j for $j \in J_k$. Then

$$\frac{1}{k-t_1+1} \sum_{j=t_1}^k \eta_j = \frac{1}{k-t_1+1} \left(\sum_{j \in J_k} \eta_j + \sum_{j \notin J_k} \eta_j \right) \\
\geq \frac{1}{k-t_1+1} \left(\eta_{mk} + \sum_{j \notin J_k} \eta_{mk} \right) \\
\geq \frac{1}{k-t_1+1} \left(\eta_{mk} + \eta_{mk} \left(k - t_1 + 1 - \left\lceil \frac{k-t_1+1}{2} \right\rceil \right) \right) \\
\geq \frac{\eta_{mk}}{k-t_1+1} \\
+ \frac{\eta_{mk}}{k-t_1+1} \left(k - t_1 + 1 - \left(\frac{k-t_1+1}{2} + 1 \right) \right) \\
= \frac{\eta_{mk}}{2}.$$

Thus, from (3.16), we have that, for all $j \in J_k$,

(3.17)
$$\eta_{j} < 2\left(\Psi(B_{t_{1}}) + M - 1 - \ln m\right) \equiv \beta_{0}'.$$

Since the term inside brackets in (3.14) is less than or equal to zero, we conclude from (3.14) and (3.17) that for all $j \in J_k$

$$-\ln\cos^2\theta_j < \beta_0'.$$

Therefore, we obtain

$$\cos \theta_j > e^{-\beta_0'/2} \equiv \beta_0,$$

which implies (3.9). Similarly, from (3.14) and (3.17), we have that for all $j \in J_k$,

$$1 - \frac{q_j}{\cos^2 \theta_j} + \ln \frac{q_j}{\cos^2 \theta_j} > -\beta_0'.$$

Note also that the function (3.15) achieves the maximum value of 0 at p=1 and satisfies $u(p) \to -\infty$ both as $p \to 0$ and $p \to \infty$. Therefore, it follows that for all $j \in J_k$

$$0 < \beta_2' \le \frac{q_j}{\cos^2 \theta_j} \le \beta_3$$

for positive constants β'_2 and β_3 . Therefore, we obtain

$$q_j \le \beta_3 \cos^2 \theta_j \le \beta_3,$$

 $q_j \ge \beta_2' \cos^2 \theta_j \ge \beta_2' \beta_0^2 \equiv \beta_2$

from which we get by using (3.2)

$$\beta_2 \le \frac{s_j^T B_j s_j}{\|s_j\|^2} \le \beta_3,$$

which implies (3.11). Finally, since

$$\frac{\|B_j s_j\|}{\|s_j\|} = \frac{q_j}{\cos \theta_j},$$

we have for $j \in J_k$

$$\frac{\|B_j s_j\|}{\|s_j\|} \le \frac{\beta_3}{\beta_0} \equiv \beta_1.$$

Therefore, the proof is complete.

By (3.12) and (3.13), we note that (3.7) and (3.8) equal

$$\gamma_k \frac{\hat{y}_k^T s_k}{\|s_k\|^2} \ge m$$
 and $\gamma_k \frac{\|\hat{y}_k\|^2}{s_k^T \hat{y}_k} \le M$.

The following theorem shows the global convergence of the msBFGS method.

Theorem 3.3. Let $\{x_k\}$ be the infinite sequence generated by the msBFGS method. Suppose that Assumption A holds. If (3.7) and (3.8) are satisfied for any $k \geq 0$, then

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

Proof. Let $K = \{k | \text{Inequalities (3.9), (3.10) and (3.11) hold}\}$. Since Lemma 3.2 holds for the case $t_1 = 0$, the set K is not empty. For the msBFGS method, Lemma 3.1 holds and the Zoutendijk condition can be written as

$$\sum_{k=0}^{\infty} (\|g_k\| \cos \theta_k)^2 < \infty.$$

Therefore, by (3.9), we obtain

$$\lim_{k \to \infty, \ k \in K} \|g_k\| = 0,$$

which implies the result.

Theorem 3.3 yields the following corollary that corresponds to the convergence result of Cheng and Li [5].

Corollary 3.4. Suppose that Assumption A and the following two assumptions hold.

- (1) The objective function f is twice continuously differentiable.
- (2) The level set Ω is convex and there exist positive constants λ_1 and λ_2 such that

$$\lambda_1 ||v||^2 \le v^T G(x) v \le \lambda_2 ||v||^2 \quad \forall x \in \Omega, v \in \mathbb{R}^n.$$

Let $\gamma_k = \frac{y_k^T s_k}{\|y_k\|^2}$, $\phi_k = 0$ and $\{x_k\}$ be the infinite sequence generated by the msBFGS method. Then

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

3.2. Superlinear convergence

Now we turn to prove the superlinear convergence of the msBFGS method. To do this, we make the following additional assumptions.

Assumption B

- (1) The function f is twice continuously differentiable in an open convex neighborhood $U(x^*)$ of x^* , where $g(x^*) = 0$ and $G(x^*)$ is positive definite.
- (2) The second derivative G is Lipschitz continuous in $U(x^*)$, i.e. there exists a constant $L_G > 0$ such that

$$(3.18) ||G(x) - G(x^*)|| \le L_G ||x - x^*||$$

holds for any x in $U(x^*)$.

- (3) $\{x_k\}$ converges to x^* .
- (4) There exist positive constants c_1 and c_2 such that $c_1 \leq \gamma_k \leq c_2$ holds for any k.

Under Assumption B(1), G(x) is uniformly positive definite for any $x \in U(x^*)$. Therefore, there is a constant m' > 0 such that for all $x \in U(x^*)$

$$(3.19) ||g(x)|| \ge m'||x - x^*||$$

and

$$(3.20) v^T G(x)v \ge m' ||v||^2 \quad \forall v \in R^n.$$

Particularly, by using the mean-value theorem, these show that for $k \geq k_0$

$$y_k^T s_k = \left(\int_0^1 G(x_k + t s_k) s_k dt\right)^T s_k \ge m' \|s_k\|^2,$$

since $x_k + ts_k \in U(x^*)$ for $k \geq k_0$, where k_0 is some nonnegative integer. Therefore, under Assumptions A and B, (3.12) and (3.13) yield that

$$\gamma_k(\rho_k^{(1)} + \phi_k) = \gamma_k \frac{\hat{y}_k^T s_k}{\|s_k\|^2}$$

$$= \gamma_k \left(\frac{y_k^T s_k}{\|s_k\|^2} + \phi_k\right)$$

$$\geq \gamma_k \left(\frac{m'\|s_k\|^2}{\|s_k\|^2} + \phi_k\right)$$

$$\geq \gamma_k (m' + \phi_k)$$

$$\geq \gamma_k m'$$

$$\geq c_1 m'$$

and

$$\frac{\gamma_k(\rho_k^{(2)} + 2\phi_k \rho_k^{(1)} + \phi_k^2)}{\rho_k^{(1)} + \phi_k} = \gamma_k \frac{\|\hat{y}_k\|^2}{\hat{y}_k^T s_k} \\
\leq \gamma_k \frac{(L_g + \phi_k)^2 \|s_k\|^2}{m' \|s_k\|^2} \\
\leq c_2 \frac{(L_g + \phi_k)^2}{m'}.$$

These imply that inequalities (3.7) and (3.8) hold for $m=c_1m', M=c_2\frac{(L_g+C)^2}{m'}$ and $t_1=k_0$. Thus, there exists a nonempty set $J_k=\{j|\text{Inequalities (3.9)},$ (3.10) and (3.11) hold, $k_0\leq j\leq k\}$ from Lemma 3.2.

Lemma 3.5. Under Assumptions A and B, we have

(3.21)
$$\sum_{k=0}^{\infty} ||x_k - x^*|| < \infty$$

and

$$(3.22) \sum_{k=0}^{\infty} \tau_k < \infty,$$

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

Proof. We can assume $k \ge k_0$ without loss of generality. It follows from (2.5) that

$$-(1 - \sigma_2)g_k^T s_k \le (g_{k+1} - g_k)^T s_k \le ||g_{k+1} - g_k|| ||s_k|| \le L_g ||s_k||^2.$$

Using (3.1) yields the relation

(3.23)
$$\frac{(1-\sigma_2)}{L_g} \|g_k\| \cos \theta_k \le \|s_k\|.$$

Since f is convex function on $U(x^*)$, we have

$$\begin{aligned}
f_k - f_* &\leq g_k^T (x_k - x^*) \\
&\leq \|g_k\| \|x_k - x^*\| \\
&\leq \frac{\|g_k\|^2}{m'},
\end{aligned}$$
(3.24)

where the last inequality follows from (3.19). For $j \in J_k$, we obtain from (2.4), (3.1) and (3.23)

$$f_{j+1} \leq f_j + \sigma_1 g_j^T s_j = f_j - \sigma_1 ||g_j|| ||s_j|| \cos \theta_j \leq f_j - \sigma_1 \frac{1 - \sigma_2}{L_a} ||g_j||^2 \cos \theta_j^2.$$

Therefore, by (3.9), we have

$$(3.25) f_j - f_{j+1} \ge \sigma_1 \beta_0^2 \frac{1 - \sigma_2}{L_q} \|g_j\|^2.$$

Letting $\eta \equiv \sigma_1 \beta_0^2 (1 - \sigma_2)/L_q$, we obtain from (3.24) and (3.25)

$$m'(f_j - f_*) \le \frac{1}{\eta}(f_j - f_{j+1}),$$

which implies

$$f_{j+1} - f_* \leq r^2 (f_j - f_*),$$

where $r \equiv \sqrt{1 - \eta m'}$. (Note that $1 > 1 - \eta m' \ge 0$ since $\{f_k\}$ is a decreasing sequence.) Since J_k has at least $\lceil (k - k_0 + 1)/2 \rceil$ elements by Lemma 3.2 and $\{f_k\}$ is decreasing, we have

$$f_{k+1} - f_* \leq (f_{j_{max}^k + 1} - f_*) \qquad (j_{max}^k \equiv \arg\max\{j | j \in J_k\})$$

$$\leq r^2 (f_{j_{max}^k} - f_*)$$

$$\leq \dots$$

$$\leq r^{2\lceil (k - k_0 + 1)/2 \rceil - 1} (f_{j_{min}^k} - f_*) \qquad (j_{min}^k \equiv \arg\min\{j | j \in J_k\})$$

$$\leq r^{2(k - k_0 + 1)/2 - 1} (f_{j_{min}^k} - f_*)$$

$$= r^{k - k_0} (f_{j_{min}^k} - f_*)$$

$$\leq r^{k - k_0} (f_{k_0} - f_*).$$

Moreover, we can derive the lower bound of $f_{k+1} - f_*$ from Taylor's expansion and (3.20) as follows

$$\frac{1}{2}m'\|x_{k+1} - x^*\|^2 \le f_{k+1} - f_*.$$

Therefore, we obtain

$$||x_{k+1} - x^*|| \leq \sqrt{\frac{2(f_{k+1} - f_*)}{m'}}$$

$$\leq \sqrt{\frac{2(f_{k_0} - f_*)r^k}{m'r^{k_0}}}$$

$$= a_1 \left(\sqrt{r}\right)^k,$$

where
$$a_1 \equiv \sqrt{\frac{2(f_{k_0} - f_*)}{m'r^{k_0}}}$$
. Hence we obtain (3.21). Finally, since $\tau_k \leq ||x_k - x^*|| + ||x_{k+1} - x^*||$, (3.22) follows from (3.21) directly.

Now, we add the following assumption.

Assumption C

The parameters γ_k and ϕ_k satisfy

(3.26)
$$\sum_{k=0}^{\infty} |\gamma_k - 1| < \infty \quad \text{and} \quad \sum_{k=0}^{\infty} \phi_k < \infty.$$

Adding Assumption C, we have the following lemma.

Lemma 3.6. Suppose that Assumptions A, B and C hold. Then there exists a sequence $\{\epsilon_k\}$ such that $\{s_k\}$ and $\{z_k\}$ satisfy for k sufficiently large

and
$$\sum_{k=0}^{\infty} \epsilon_k < \infty$$
 holds.

Proof. Using (3.18), we have

$$\begin{split} &\|\gamma_{k}\hat{y}_{k}-G(x^{*})s_{k}\|\\ &\leq\|(\gamma_{k}-1)\hat{y}_{k}\|+\|y_{k}+\phi_{k}s_{k}-G(x^{*})s_{k}\|\\ &\leq|\gamma_{k}-1|\|\hat{y}_{k}\|+\int_{0}^{1}\|G(x_{k}+ts_{k})-G(x^{*})\|dt\|s_{k}\|+\|\phi_{k}s_{k}\|\\ &\leq|\gamma_{k}-1|\|\hat{y}_{k}\|+\int_{0}^{1}\|x_{k}+ts_{k}-x^{*}\|dtL_{G}\|s_{k}\|+\|\phi_{k}s_{k}\|\\ &\leq|\gamma_{k}-1|\|\hat{y}_{k}\|+\int_{0}^{1}(\|t(x_{k+1}-x^{*})\|+\|(1-t)(x_{k}-x^{*})\|)dtL_{G}\|s_{k}\|\\ &+\|\phi_{k}s_{k}\|\\ &=|\gamma_{k}-1|\|\hat{y}_{k}\|+\frac{1}{2}(\|x_{k+1}-x^{*}\|+\|x_{k}-x^{*}\|)L_{G}\|s_{k}\|+\|\phi_{k}s_{k}\|\\ &\leq|\gamma_{k}-1|\|\hat{y}_{k}\|+\max\{\|x_{k+1}-x^{*}\|,\|x_{k}-x^{*}\|\}L_{G}\|s_{k}\|+\|\phi_{k}s_{k}\|\\ &\leq|\gamma_{k}-1|(\|y_{k}\|+\|\phi_{k}s_{k}\|)+(L_{G}\tau_{k}+\phi_{k})\|s_{k}\|\\ &\leq(|\gamma_{k}-1|(L_{q}+\phi_{k})+L_{G}\tau_{k}+\phi_{k})\|s_{k}\|. \end{split}$$

Therefore, (3.27) holds for
$$\epsilon_k = |\gamma_k - 1| (L_g + \phi_k) + L_G \tau_k + \phi_k$$
, and $\sum_{k=0}^{\infty} \epsilon_k < \infty$ follows from (3.22) and (3.26).

Moreover, we give the following lemma to show the convergence property. This lemma was shown by Dennis and Moré [6].

Lemma 3.7. Let $f: R^n \to R$ be twice differentiable in an open convex set D in R^n , and assume that for some \hat{x} in D, G is continuous at \hat{x} and $G(\hat{x})$ is nonsingular. Let $\{B_k\}$ in $R^{n\times n}$ be a sequence of nonsingular matrices and suppose that for some x_0 in D, the sequence $\{x_k\}$ generated by

$$x_{k+1} = x_k - B_k^{-1} g_k$$

remains in D and converges to \hat{x} . Then the sequence $\{x_k\}$ converges Q-superlinearly to \hat{x} and $g(\hat{x}) = 0$ if and only if

(3.28)
$$\lim_{k \to \infty} \frac{\|(B_k - G(\hat{x}))(x_{k+1} - x_k)\|}{\|x_{k+1} - x_k\|} = 0.$$

Note that (3.28) is called the Dennis-Moré condition. From Lemma 3.7, we obtain the next theorem.

Theorem 3.8. Let the sequences $\{x_k\}$ and $\{B_k\}$ be generated by the msBFGS method. Suppose that Assumptions A, B and C hold. Then

(3.29)
$$\lim_{k \to \infty} \frac{\|(B_k - G(x^*))s_k\|}{\|s_k\|} = 0$$

holds and the sequence $\{\|B_k^{-1}\|\}$ is bounded. Moreover, if the parameter σ_1 in (2.4) is chosen to satisfy $\sigma_1 \in (0, \frac{1}{2})$, then the sequence $\{x_k\}$ converges to x^* superlinealy.

Proof. Let us define

(3.30)
$$\tilde{s}_k = G(x^*)^{\frac{1}{2}} s_k, \quad \tilde{z}_k = G(x^*)^{-\frac{1}{2}} z_k,$$

(3.31)
$$\tilde{B}_{k} = G(x^{*})^{-\frac{1}{2}} B_{k} G(x^{*})^{-\frac{1}{2}},$$

$$\cos \tilde{\theta}_{k} = \frac{\tilde{s}_{k}^{T} \tilde{B}_{k} \tilde{s}_{k}}{\|\tilde{B}_{k} \tilde{s}_{k}\| \|\tilde{s}_{k}\|}$$

and

$$\tilde{q}_k = \frac{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k}{\|\tilde{s}_k\|^2}.$$

Though the first part of this theorem can be shown in the same way as the proof of Theorem 3.2 in [4], we do not omit the proof for readability. From (2.6), (3.30) and (3.31), it follows that

$$\tilde{B}_{k+1} = \tilde{B}_k - \frac{\tilde{B}_k \tilde{s}_k \tilde{s}_k^T \tilde{B}_k}{\tilde{s}_k^T \tilde{B}_k \tilde{s}_k} + \frac{\tilde{z}_k \tilde{z}_k^T}{\tilde{z}_k^T \tilde{s}_k}.$$

Thus, we obtain, just as in (3.5)

$$(3.32) \qquad \Psi(\tilde{B}_{k+1}) = \Psi(\tilde{B}_{k}) + \frac{\|\tilde{z}_{k}\|^{2}}{\tilde{s}_{k}^{T}\tilde{z}_{k}} - \ln\frac{\tilde{s}_{k}^{T}\tilde{z}_{k}}{\|\tilde{s}_{k}\|^{2}} + \ln\cos^{2}\tilde{\theta}_{k} - 1 + \left(1 - \frac{\tilde{q}_{k}}{\cos^{2}\tilde{\theta}_{k}} + \ln\frac{\tilde{q}_{k}}{\cos^{2}\tilde{\theta}_{k}}\right).$$

For k sufficiently large, it follows from (3.27) that

where $\bar{c} = ||G(x^*)^{-\frac{1}{2}}||^2$. Using the triangle inequality yields

$$\|\tilde{z}_k - \tilde{s}_k\| \ge \|\tilde{z}_k\| - \|\tilde{s}_k\|$$

and

$$\|\tilde{z}_k - \tilde{s}_k\| = \|\tilde{s}_k - \tilde{z}_k\| \ge \|\tilde{s}_k\| - \|\tilde{z}_k\|.$$

So we have

$$(3.34) (1 - \bar{c}\epsilon_k) \|\tilde{s}_k\| \le \|\tilde{z}_k\| \le (1 + \bar{c}\epsilon_k) \|\tilde{s}_k\|.$$

From (3.33) and (3.34), it follows that

$$\|\tilde{z}_k\|^2 - 2\tilde{z}_k^T \tilde{s}_k + \|\tilde{s}_k\|^2 \le \bar{c}^2 \epsilon_k^2 \|\tilde{s}_k\|^2$$

and

$$(1 - \bar{c}\epsilon_k)^2 \|\tilde{s}_k\|^2 - 2\tilde{z}_k^T \tilde{s}_k + \|\tilde{s}_k\|^2 \le \|\tilde{z}_k\|^2 - 2\tilde{z}_k^T \tilde{s}_k + \|\tilde{s}_k\|^2,$$

from which we get

$$(3.35) (1 - \bar{c}\epsilon_k)^2 \|\tilde{s}_k\|^2 - 2\tilde{z}_k^T \tilde{s}_k + \|\tilde{s}_k\|^2 \le \bar{c}^2 \epsilon_k^2 \|\tilde{s}_k\|^2.$$

By (3.35), we have

$$(3.36) \frac{\tilde{z}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} \ge 1 - \bar{c}\epsilon_k.$$

Since $\tilde{z}_k^T \tilde{s}_k > 0$ is satisfied, (3.34) yields

(3.37)
$$\frac{\|\tilde{z}_k\|^2}{\tilde{z}_k^T \tilde{s}_k} \le (1 + \bar{c}\epsilon_k)^2 \frac{\|\tilde{s}_k\|^2}{\tilde{z}_k^T \tilde{s}_k}.$$

By using the fact $\sum_{k=0}^{\infty} \epsilon_k < \infty$, there exists an integer \bar{k} such that $\bar{c}\epsilon_k \leq \frac{1}{2}$ for $k \geq \bar{k}$. Therefore, it follows from (3.36) and (3.37) for $k \geq \bar{k}$ that

$$(3.38) \qquad \frac{\|\tilde{z}_{k}\|^{2}}{\tilde{z}_{k}^{T}\tilde{s}_{k}} \leq (1+\bar{c}\epsilon_{k})^{2} \frac{\|\tilde{s}_{k}\|^{2}}{\tilde{z}_{k}^{T}\tilde{s}_{k}}$$

$$\leq (1+\bar{c}\epsilon_{k}) \frac{1+\bar{c}\epsilon_{k}}{1-\bar{c}\epsilon_{k}}$$

$$= 1+\epsilon_{k} \left(\frac{2\bar{c}}{1-\bar{c}\epsilon_{k}}+\bar{c}+\frac{2\bar{c}^{2}\epsilon_{k}}{1-\bar{c}\epsilon_{k}}\right)$$

$$\leq 1+\epsilon_{k} \left(\frac{2\bar{c}}{1-\frac{1}{2}}+\bar{c}+\frac{2\bar{c}\frac{1}{2}}{1-\frac{1}{2}}\right)$$

$$= 1+7\bar{c}\epsilon_{k}.$$

We notice that the inequality $-\ln(1-x) \le 2x$ holds for $0 < x \le \frac{1}{2}$. So it follows from (3.36)

$$(3.39) -\ln \frac{\tilde{z}_k^T \tilde{s}_k}{\|\tilde{s}_k\|^2} \le -\ln(1 - \bar{c}\epsilon_k) \le 2\bar{c}\epsilon_k.$$

Thus, by (3.32), (3.38) and (3.39), for $k \ge \bar{k}$ we have

$$\Psi(\tilde{B}_{k+1}) \le \Psi(\tilde{B}_k) + 9\bar{c}\epsilon_k + \ln\cos^2\tilde{\theta}_k + \left(1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right).$$

Hence by using (3.32) again, there is a positive constant \hat{c} such that

$$(3.40) \quad \Psi(\tilde{B}_{k+1})$$

$$\leq \Psi(\tilde{B}_{\bar{k}}) + \sum_{j=\bar{k}}^{k} \left(9\bar{c}\epsilon_{j} + \ln\cos^{2}\tilde{\theta}_{j} + \left(1 - \frac{\tilde{q}_{j}}{\cos^{2}\tilde{\theta}_{j}} + \ln\frac{\tilde{q}_{j}}{\cos^{2}\tilde{\theta}_{j}} \right) \right)$$

$$= \Psi(\tilde{B}_{\bar{k}-1}) + \frac{\|\tilde{z}_{\bar{k}-1}\|^{2}}{\tilde{s}_{\bar{k}-1}^{T}\tilde{z}_{\bar{k}-1}} - \ln\frac{\tilde{s}_{\bar{k}-1}^{T}\tilde{z}_{\bar{k}-1}}{\|\tilde{s}_{\bar{k}-1}\|^{2}} + \ln\cos^{2}\tilde{\theta}_{\bar{k}-1} - 1$$

$$+ \left(1 - \frac{\tilde{q}_{\bar{k}-1}}{\cos^{2}\tilde{\theta}_{\bar{k}-1}} + \ln\frac{\tilde{q}_{\bar{k}-1}}{\cos^{2}\tilde{\theta}_{\bar{k}-1}} \right)$$

$$+ \sum_{j=\bar{k}}^{k} \left(9\bar{c}\epsilon_{j} + \ln\cos^{2}\tilde{\theta}_{j} + \left(1 - \frac{\tilde{q}_{j}}{\cos^{2}\tilde{\theta}_{j}} + \ln\frac{\tilde{q}_{j}}{\cos^{2}\tilde{\theta}_{j}} \right) \right)$$

$$\begin{split} &= \Psi(\tilde{B}_{\bar{k}-1}) + \sum_{j=\bar{k}-1}^{k} \left(\ln \cos^{2} \tilde{\theta}_{j} + 1 - \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + \ln \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + 9\bar{c}\epsilon_{j} \right) \\ &+ \sum_{j=\bar{k}-1}^{\bar{k}-1} \left(-9\bar{c}\epsilon_{j} + \frac{\|\tilde{z}_{j}\|^{2}}{\tilde{s}_{j}^{T}\tilde{z}_{j}} - \ln \frac{\tilde{s}_{j}^{T}\tilde{z}_{j}}{\|\tilde{s}_{j}\|^{2}} - 1 \right) \\ &= \Psi(\tilde{B}_{\bar{k}-2}) + \sum_{j=\bar{k}-2}^{k} \left(\ln \cos^{2} \tilde{\theta}_{j} + 1 - \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + \ln \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + 9\bar{c}\epsilon_{j} \right) \\ &+ \sum_{j=\bar{k}-2}^{\bar{k}-1} \left(-9\bar{c}\epsilon_{j} + \frac{\|\tilde{z}_{j}\|^{2}}{\tilde{s}_{j}^{T}\tilde{z}_{j}} - \ln \frac{\tilde{s}_{j}^{T}\tilde{z}_{j}}{\|\tilde{s}_{j}\|^{2}} - 1 \right) \\ &= \dots \\ &= \Psi(\tilde{B}_{0}) + \sum_{j=0}^{k} \left(\ln \cos^{2} \tilde{\theta}_{j} + 1 - \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + \ln \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + 9\bar{c}\epsilon_{j} \right) \\ &+ \sum_{j=0}^{\bar{k}-1} \left(-9\bar{c}\epsilon_{j} + \frac{\|\tilde{z}_{j}\|^{2}}{\tilde{s}_{j}^{T}\tilde{z}_{j}} - \ln \frac{\tilde{s}_{j}^{T}\tilde{z}_{j}}{\|\tilde{s}_{j}\|^{2}} - 1 \right) \\ &= \Psi(\tilde{B}_{0}) + \sum_{j=0}^{k} \left(\ln \cos^{2} \tilde{\theta}_{j} + 1 - \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + \ln \frac{\tilde{q}_{j}}{\cos^{2} \tilde{\theta}_{j}} + 9\bar{c}\epsilon_{j} \right) + \hat{c}. \end{split}$$

Furthermore, similar comments to those for (3.4) and (3.15) indicate

(3.41)
$$\Psi(\tilde{B}_{k+1}) \ge n \quad \text{and} \quad 1 - \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} + \ln \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} \le 0.$$

From (3.40), (3.41), the expressions $\ln \cos^2 \tilde{\theta}_j \leq 0$ and $\sum_{k=0}^{\infty} \epsilon_k < \infty$, we see that $\{\Psi(\tilde{B}_k)\}$ is bounded, and since

$$n - \sum_{j=0}^{k} \left(\ln \cos^2 \tilde{\theta}_j + 1 - \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} + \ln \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} \right) \le \Psi(\tilde{B}_0) + \sum_{j=0}^{k} 9\bar{c}\epsilon_j + \hat{c},$$

we have

$$0 \le -\sum_{j=0}^{k} \left(\ln \cos^2 \tilde{\theta}_j + 1 - \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} + \ln \frac{\tilde{q}_j}{\cos^2 \tilde{\theta}_j} \right) < \infty.$$

So we obtain

$$(3.42) \ln \cos \tilde{\theta}_k \to 0$$

and

$$(3.43) 1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \to 0.$$

Expression (3.42) implies

(3.44)
$$\cos \tilde{\theta}_k \to 1.$$

Furthermore, since (3.43) and the comments following (3.15) show $\frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} \to 1$, (3.44) implies

$$(3.45) \tilde{q}_k \to 1.$$

Now it follows from (3.44) and (3.45) that

$$\frac{\|(B_k - G(x^*))s_k\|^2}{\|s_k\|^2} \frac{1}{\|G(x^*)^{\frac{1}{2}}\|^4} \leq \frac{\|(B_k - G(x^*))s_k\|^2}{\|G(x^*)^{\frac{1}{2}}s_k\|^2 \|G(x^*)^{\frac{1}{2}}\|^2} \\
\leq \frac{\|G(x^*)^{-\frac{1}{2}}(B_k - G(x^*))s_k\|^2}{\|G(x^*)^{\frac{1}{2}}s_k\|^2} \\
= \frac{\|(\tilde{B}_k - I)\tilde{s}_k\|^2}{\|\tilde{s}_k\|^2} \\
= \frac{\|\tilde{B}_k\tilde{s}_k\|^2 - 2\tilde{s}_k^T\tilde{B}_k\tilde{s}_k + \|\tilde{s}_k\|^2}{\|\tilde{s}_k\|^2} \\
= \frac{\tilde{q}_k^2}{\cos^2\tilde{\theta}_k} - 2\tilde{q}_k + 1 \to 0,$$

which implies (3.29). Since $\{\Psi(\tilde{B}_k)\}$ is bounded, (3.4) implies that there is a positive constant P such that for all k

$$P \ge \sum_{j=1}^{n} (\tilde{\mu}_{k,j} - \ln \tilde{\mu}_{k,j}) > 0,$$

where $0 < \tilde{\mu}_{k,1} \le \cdots \le \tilde{\mu}_{k,n}$ are the eigenvalues of \tilde{B}_k . Since this means $P \ge \tilde{\mu}_{k,j} - \ln \tilde{\mu}_{k,j} > 0$ for all $1 \le j \le n$, there exist positive constants p_1 and p_2 such that

$$p_1 \leq \tilde{\mu}_{k,j} \leq p_2$$
 for all $1 \leq j \leq n$,

where p_1 and p_2 satisfy $p_1 - \ln p_1 = P$ and $p_2 - \ln p_2 = P$. So we get

$$\|\tilde{B}_k^{-1}\|_2 = \sqrt{\rho(\tilde{B}_k^{-T}\tilde{B}_k^{-1})} = \sqrt{\rho\left((\tilde{B}_k^{-1})^2\right)} = \frac{1}{\tilde{\mu}_{k,1}} \le \frac{1}{p_1},$$

where $\rho(A)$ denotes the spectral radius of the matrix A. Therefore, the upper bound of $||B_k^{-1}||$ is estimated by

$$||B_{k}^{-1}|| = ||G(x^{*})^{-\frac{1}{2}}G(x^{*})^{\frac{1}{2}}B_{k}^{-1}G(x^{*})^{\frac{1}{2}}G(x^{*})^{-\frac{1}{2}}||$$

$$\leq ||G(x^{*})^{-\frac{1}{2}}||^{2}||(G(x^{*})^{-\frac{1}{2}}B_{k}G(x^{*})^{-\frac{1}{2}})^{-1}||$$

$$\leq ||G(x^{*})^{-\frac{1}{2}}||^{2}||\tilde{B}_{k}^{-1}||.$$

Next we verify that $\alpha_k=1$ is accepted for all k sufficiently large. Since $\|d_k\|=\|B_k^{-1}g_k\|\leq \|B_k^{-1}\|\|g_k\|\to 0$ from the boundedness of $\|B_k^{-1}\|$ and Assumptions B(1) and B(3), by Taylor's expansion we obtain

$$f(x_k + d_k) - f(x_k) - \sigma_1 g_k^T d_k = (1 - \sigma_1) g_k^T d_k + \frac{1}{2} d_k^T G(x_k + t d_k) d_k$$

$$= -(1 - \sigma_1) d_k^T B_k d_k + \frac{1}{2} d_k^T G(x_k + t d_k) d_k$$

$$= -\left(\frac{1}{2} - \sigma_1\right) d_k^T G(x^*) d_k + o(\|d_k\|^2),$$

where $t \in (0,1)$ and the last equality follows from (3.29). Thus, $f(x_k + d_k) - f(x_k) - \sigma_1 g_k^T d_k \leq 0$ is satisfied for all k sufficiently large. This means that $\alpha_k = 1$ satisfies (2.4) for all k sufficiently large. On the other hand, we have

$$g(x_k + d_k)^T d_k - \sigma_2 g_k^T d_k = (g(x_k + d_k) - g_k)^T d_k + (1 - \sigma_2) g_k^T d_k$$

= $d_k^T G(x_k + t d_k) d_k - (1 - \sigma_2) d_k^T B_k d_k$
= $\sigma_2 d_k^T G(x^*) d_k + o(\|d_k\|^2),$

where $t \in (0,1)$. Thus, we have $g(x_k + d_k)^T d_k \ge \sigma_2 g_k^T d_k$, which means that $\alpha_k = 1$ satisfies (2.5) for all k sufficiently large. From Lemma 3.7 and (3.29), we can deduce that the sequence $\{x_k\}$ converges superlinearly to x^* .

§4. Practical choices of γ_k

In this section, we propose three kinds of scaling factors for the msBFGS method and show the convergence properties with them, respectively. The convergence properties of the msBFGS method depend on the choices of γ_k and ϕ_k . For the global convergence, it is important to choose γ_k and ϕ_k that satisfy (3.7) and (3.8), and for the superlinear convergence, it is important to choose them that satisfy (3.26). Li and Fukushima [9] suggested that one of suitable choices of ϕ_k for the msBFGS method with $\gamma_k = 1$ is

$$\phi_k = \delta_k \|g_k\|,$$

where $\delta_k \in [\underline{\delta}, \overline{\delta}]$ ($\underline{\delta}$ and $\overline{\delta}$ are positive constants). This choice may be also efficient for the convergence properties of the msBFGS method with $\gamma_k \neq 1$. Therefore, we choose ϕ_k in (4.1).

Now, we propose three kinds of scaling factors as follows:

(i) Let D_k be some scaling matrix for \bar{G}_k . Then, we expect that the ms-BFGS method with B_k which approximates to $D_k\bar{G}_k$ has a numerical stability. Such D_k must be the matrix which is a rough approximation to \bar{G}_k^{-1} . Thus, we require the relation $D_{k+1}\hat{y}_k \approx s_k$. Let $D_{k+1} = \gamma_k I$ for simplicity. By minimizing the norms $\|s_k - \gamma_k \hat{y}_k\|$ and $\|\frac{1}{\gamma_k} s_k - \hat{y}_k\|$, we have

$$\gamma_k^{(1)} = rac{\hat{y}_k^T s_k}{\|\hat{y}_k\|^2}$$
 and $\gamma_k^{(2)} = rac{\|s_k\|^2}{\hat{y}_k^T s_k}$,

respectively. Now, we propose the first scaling factor by using the convex combination of $\gamma_k^{(1)}$ and $\gamma_k^{(2)}$ as follows

(4.2)
$$\gamma_k = (1 - t)\gamma_k^{(1)} + t\gamma_k^{(2)},$$

where $t \in [0,1]$. If the Wolfe conditions (2.4) and (2.5) are satisfied, then $\hat{y}_k^T s_k > 0$ holds. Thus, γ_k in (4.2) is always positive, which implies that the msBFGS method with (4.1) and (4.2) generates a descent search direction. For the msBFGS method with (4.1) and (4.2), we obtain the following convergence theorem.

Theorem 4.1. Let ϕ_k and γ_k be defined by (4.1) and (4.2), respectively. Let $\{x_k\}$ be the infinite sequence generated by the msBFGS method. Suppose that Assumption A holds. Then

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

Proof. To prove this theorem by contradiction, we assume that there is a constant $\varepsilon > 0$ such that $||g_k|| \ge \varepsilon$ for all k. Since d_k is a descent search direction and (2.4) is satisfied, we have $x_k \in \Omega$ for all k. Thus, from Assumption A, $||g_k||$ is bounded above. Therefore, $\phi_k(=\delta_k||g_k||)$ is included in a bounded interval [0, C] for some C > 0. We note that

$$(4.3) \quad \hat{y}_k^T s_k = y_k^T s_k + \phi_k \|s_k\|^2 \ge \phi_k \|s_k\|^2 = \delta_k \|g_k\| \|s_k\|^2 \ge \underline{\delta} \varepsilon \|s_k\|^2.$$

From (3.12) and (4.3), we have

$$\gamma_{k}(\rho_{k}^{(1)} + \phi_{k}) = \gamma_{k} \frac{\hat{y}_{k}^{T} s_{k}}{\|s_{k}\|^{2}} \\
= (1 - t) \frac{(\hat{y}_{k}^{T} s_{k})^{2}}{\|\hat{y}_{k}\|^{2} \|s_{k}\|^{2}} + t \\
\geq (1 - t) \frac{(\underline{\delta} \varepsilon \|s_{k}\|^{2})^{2}}{(L_{g} + C)^{2} \|s_{k}\|^{4}} + t \\
\geq (1 - t) \frac{(\underline{\delta} \varepsilon)^{2}}{(L_{g} + C)^{2}} + t \\
\geq \min \left\{ \frac{(\underline{\delta} \varepsilon)^{2}}{(L_{g} + C)^{2}}, 1 \right\}$$

and by (3.13) and (4.3), we obtain

$$\frac{\gamma_k(\rho_k^{(2)} + 2\phi_k \rho_k^{(1)} + \phi_k^2)}{\rho_k^{(1)} + \phi_k} = \gamma_k \frac{\|\hat{y}_k\|^2}{\hat{y}_k^T s_k}
= (1 - t) + t \frac{\|s_k\|^2 \|\hat{y}_k\|^2}{(\hat{y}_k^T s_k)^2}
\leq (1 - t) + t \frac{(L_g + C)^2 \|s_k\|^4}{(\underline{\delta}\varepsilon)^2 \|s_k\|^4}
\leq (1 - t) + t \frac{(L_g + C)^2}{(\underline{\delta}\varepsilon)^2}
\leq \max \left\{ 1, \frac{(L_g + C)^2}{(\underline{\delta}\varepsilon)^2} \right\}.$$

These imply that inequalities (3.7) and (3.8) hold with $m=\min\left\{\frac{(\delta\varepsilon)^2}{(L_g+C)^2},1\right\}$ and $M=\max\left\{1,\frac{(L_g+C)^2}{(\underline{\delta\varepsilon})^2}\right\}$ for any $k\geq 0$. Thus, it follows from Theorem 3.3 that $\liminf_{k\to\infty}\|g_k\|=0$, which yields a contradiction. Therefore, the theorem is proved.

(ii) Next, we give another scaling factor. Powell [15] indicated that the BFGS method suffers more from large eigenvalues of B_k than from small ones (see also [16]). Thus, we choose

(4.4)
$$\gamma_{k}' = \left(-l + \frac{\|B_{k}s_{k}\|^{2}}{s_{k}^{T}B_{k}s_{k}}\right) \frac{\hat{y}_{k}^{T}s_{k}}{\|\hat{y}_{k}\|^{2}},$$

where l is a positive constant, because taking the trace in the msBFGS formula

with γ'_k , we have

$$\text{Tr}(B_{k+1}) = \text{Tr}(B_k) - \frac{\|B_k s_k\|^2}{s_k^T B_k s_k} + \gamma_k' \frac{\|\hat{y}_k\|^2}{\hat{y}_k^T s_k}$$

$$= \text{Tr}(B_k) - l.$$

This equality shows that the msBFGS update with γ'_k can decrease the sum of eigenvalues by -l. Thus, this choice may influence the performance well. However, we can not obtain the convergence property of the msBFGS method with γ'_k and ϕ_k in (4.1) by using Theorem 3.3. Hence, for given ϕ_k , we propose the modified version of (4.4)

$$\gamma_{k}'(\rho_{k}^{(1)} + \phi_{k}) \ge \underline{m} \\
\gamma_{k}' \quad \text{if} \quad \text{and} \\
\gamma_{k}'(\rho_{k}^{(2)} + 2\phi_{k}\rho_{k}^{(1)} + \phi_{k}^{2}) \le \overline{M}(\rho_{k}^{(1)} + \phi_{k}), \\
1 \quad \text{otherwise,}$$

where \underline{m} and \overline{M} are positive constants. If the Wolfe conditions are satisfied, then $\rho_k^{(1)} \geq 0$ holds and then γ_k in (4.5) is always positive. Therefore, the msBFGS method with (4.1) and (4.5) generates a descent search direction.

The following theorem shows the global convergence of the msBFGS method with (4.1) and (4.5).

Theorem 4.2. Let ϕ_k and γ_k be defined by (4.1) and (4.5), respectively. Let $\{x_k\}$ be the infinite sequence generated by the msBFGS method. Suppose that Assumption A holds. Then

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

Proof. To prove this theorem by contradiction, we assume that there is a constant $\varepsilon > 0$ such that $||g_k|| \ge \varepsilon$ for all k. For the case $\gamma_k = 1$, expressions (3.12) and (4.3) yield

$$\gamma_k(\rho_k^{(1)} + \phi_k) = \frac{\hat{y}_k^T s_k}{\|s_k\|^2} \ge \underline{\delta}\varepsilon$$

and equation (3.13) implies

$$\frac{\gamma_{k}(\rho_{k}^{(2)} + 2\phi_{k}\rho_{k}^{(1)} + \phi_{k}^{2})}{\rho_{k}^{(1)} + \phi_{k}} = \frac{\|\hat{y}_{k}\|^{2}}{\hat{y}_{k}^{T}s_{k}} \\
\leq \frac{(L_{g} + C)^{2}\|s_{k}\|^{2}}{\underline{\delta}\varepsilon\|s_{k}\|^{2}} \\
= \frac{(L_{g} + C)^{2}}{\delta\varepsilon}.$$

Thus, these imply that inequalities (3.7) and (3.8) hold with $m = \min \{\underline{\delta}\varepsilon, \underline{\mathbf{m}}\}$ and $M = \max \{\frac{(L_g + C)^2}{\underline{\delta}\varepsilon}, \overline{M}\}$ for any k. It follows from Theorem 3.3 that $\liminf_{k \to \infty} \|g_k\| = 0$, which yields a contradiction. Therefore, the theorem is proved.

(iii) The msBFGS methods with the above two scaling factors (4.2) and (4.5) have the global convergence properties, but do not necessarily have the superlinear convergence. To establish the superlinear convergence, we propose the following scaling factor based on (4.2):

(4.6)
$$\gamma_k = \begin{cases} (1-t)\gamma_k^{(1)} + t\gamma_k^{(2)} & \text{if } ||g_k||_{\infty} > \xi, \\ 1 & \text{otherwise,} \end{cases}$$

where $t \in [0, 1]$ and ξ is a positive constant. If the Wolfe conditions are satisfied, then $\hat{y}_k^T s_k > 0$ holds. Therefore, γ_k in (4.6) is always positive. Finally, we show the global and superlinear convergence of the msBFGS method with (4.1) and (4.6).

Theorem 4.3. Let ϕ_k and γ_k be defined by (4.1) and (4.6), respectively. Let $\{x_k\}$ be the infinite sequence generated by the msBFGS method. Suppose that Assumption A holds. Then

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

In addition, if Assumptions B(1)-(3) hold and the parameter σ_1 in (2.4) is chosen to satisfy $\sigma_1 \in (0, \frac{1}{2})$, then the sequence $\{x_k\}$ converges to x^* superlinealy.

Proof. To prove the first part of this theorem by contradiction, we assume that there is a constant $\varepsilon>0$ such that $\|g_k\|\geq \varepsilon$ holds for all k. For the case $\gamma_k=(1-t)\gamma_k^{(1)}+t\gamma_k^{(2)}$, the proof of Theorem 4.1 implies that (3.7) and (3.8) hold for $m=\min\left\{\frac{(\underline{\delta}\varepsilon)^2}{(L_g+C)^2},1\right\}$ and $M=\max\left\{1,\frac{(L_g+C)^2}{(\underline{\delta}\varepsilon)^2}\right\}$. Similarly, for the case $\gamma_k=1$, the proof of Theorem 4.2 implies that (3.7) and (3.8) hold for $m=\underline{\delta}\varepsilon$ and $M=\frac{(L_g+C)^2}{\underline{\delta}\varepsilon}$. Therefore, the msBFGS method with ϕ_k in (4.1) and γ_k in (4.6) satisfy (3.7) and (3.8) for $m=\min\left\{\underline{\delta}\varepsilon,\frac{(\underline{\delta}\varepsilon)^2}{(L_g+C)^2},1\right\}$ and $M=\max\left\{\frac{(L_g+C)^2}{\underline{\delta}\varepsilon},\frac{(L_g+C)^2}{(\underline{\delta}\varepsilon)^2},1\right\}$ for any k. Thus, it follows from Theorem 3.3 that $\liminf_{k\to\infty}\|g_k\|=0$, which yields a contradiction. Therefore, we obtain the first result.

In addition, suppose that Assumptions B(1)-(3) hold. Assumptions B(1) and B(3) imply that $\gamma_k = 1$ holds for k sufficiently large. Thus, Assumption B(4) is fulfilled and we get $\sum_{k=0}^{\infty} |\gamma_k - 1| < \infty$. Since Assumptions A and B

hold, it follows from Lemma 3.5 that $\sum_{k=0}^{\infty} ||x_k - x^*|| < \infty$ is satisfied. Thus, the relation

$$\phi_k = \delta_k ||g_k|| \le \bar{\delta} ||g_k - g(x^*)|| \le \bar{\delta} L_q ||x_k - x^*||$$

yields

$$\sum_{k=0}^{\infty} \phi_k < \infty.$$

It follows that $\{\gamma_k\}$ and $\{\phi_k\}$ satisfy (3.26), i.e., Assumption C is fulfilled. Therefore, from Theorem 3.8, we obtain the superlinear convergence.

§5. Numerical experiments

In this section, we show some numerical experiments. We used the 132 nonlinear unconstrained optimization problems in the CUTEr library [3]. We chose the test problems whose dimensions were between 499 and 1000. In Table 1, we give the methods examined in our experiments.

Table 1. Methods examined in our experiments

		1
Method number	Method name	Note
(1)	${ m msBFGS}$	use ϕ_k in (4.1) and γ_k in (4.2)
(2)	${ m msBFGS}$	use ϕ_k in (4.1) and γ_k in (4.5)
(3)	${ m msBFGS}$	use ϕ_k in (4.1) and γ_k in (4.6)
(4)	standard BFGS	
(5)	sized BFGS	size B_0 by w_0^{IOL}
(6)	spectral scaling BFGS	Cheng and Li [5]

In order to compare the proposed method with some existing BFGS type methods, we tested the standard BFGS, sized BFGS method, spectral scaling BFGS method and the msBFGS method based on (4.1), (4.2), (4.5) and (4.6). We number from (1) to (6) in Table 1. we tested the sized BFGS method (Method (5)) in which we sized B_0 only at the first iteration by the inverse Oren - Luenberger parameter $\omega_0^{IOL} = \frac{y_0 B_0^{-1} y_0}{y_0^T s_0}$. The spectral scaling BFGS method (Method (6)) corresponds to Method (1) with $\phi_k = 0$ and t = 0, which is the Cheng - Li method.

All codes were written in C and run on a PC with 3.40 GHz CPU processor, 2.0GB RAM memory, and Linux operating system. We show the numerical results in Figures 1-5. In Figures 1-3, we stopped the iteration if the inequality

$$||g_k||_{\infty} \le 10^{-6}$$

was satisfied, or if CPU time exceeded 600 seconds, and in Figures 4 and 5, we stopped the iteration if the inequality

$$||q_k||_{\infty} \le 10^{-8}$$

was satisfied or if CPU time exceeded 600 seconds. For all examined methods, we chose the initial matrix $B_0 = I$. For each method, to get the search direction d_k , we did not solve the linear system of equations $B_k d_k = -g_k$. Instead we used the inverse updating formula as follows

$$H_{k+1} = H_k - \frac{H_k \hat{y}_k s_k^T + s_k (H_k \hat{y}_k)^T}{\hat{y}_k^T s_k} + \left(\frac{1}{\gamma_k} + \frac{\hat{y}_k^T H_k \hat{y}_k}{\hat{y}_k^T s_k}\right) \frac{s_k s_k^T}{\hat{y}_k^T s_k}.$$

In the line search, the step size α_k was obtained so as to satisfy the Wolfe conditions:

$$f(x_k + \alpha_k d_k) \le f(x_k) + \sigma_1 \alpha_k g_k^T d_k,$$

$$g(x_k + \alpha_k d_k)^T d_k \ge \sigma_2 g_k^T d_k,$$

where we chose $\sigma_1 = 10^{-3}$ and $\sigma_2 = 0.5$.

We adopt the performance profiles by Dolan and Moré [8] to compare the performance of the methods based on the CPU time. We introduce the performance profile by Dolan and Moré. We assume that we are concerned with the set of solvers S, which has n_s solvers, and the test set P, which has n_p problems. For each problem p and solver s, let us define

 $t_{p,s} =$ computing time required to solve problem p by solver s,

$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,s} : s \in S\}}$$

and

$$\rho_s(\nu) = \frac{1}{n_p} \left| \left\{ p \in P : r_{p,s} \le \nu \right\} \right|.$$

The function $\rho_s(\nu)$ is the probability for solver $s \in S$ that a performance ratio $r_{p,s}$ is within a factor $\nu \in R$ of the best performance ratio. In Figures 1, 2 and 3, the function $\rho_s(\nu)$ distributes the curve, and the top curve is the method which solved the most problems in a result that is within a factor ν of the best result.

Table 2. The parameter in a premiumary experiment		
Method number	Values of parameters	
(1)	$t \in \{0, 0.25, 0.5, 0.75, 1\}, \delta_k \in [0, 10]$	
(2)	$l \in \{10^{-2}, 10^{-1}, 1, 10\}, \underline{m}, \bar{M} \in [10^{-7}, 10^7], \delta_k \in [0, 10]$	
(3)	$t \in \{0, 0.25, 0.5, 0.75, 1\}, \xi \in [10^{-2}, 10^2], \delta_k \in [0, 10]$	

Table 2. The parameter in a preliminary experiment

As a preliminary experiment, we chose the value of parameter for Method (1), (2), (3) in Table 2. In Figure 1, we examine Method (1) in which we always choose t=1 and vary the value of δ_k . Figure 1 implies that Method (1) with t=1 has the tendency that the choice of the small value for δ_k performs well. In our experiments, Methods (1), (2) and (3) have the similar tendency. However, the influence of δ_k is different a little for each method. As shown in Figure 1, in some methods, by letting δ_k be a small positive value, the performance becomes rather better than the case $\delta_k = 0$. Meanwhile, in some methods, even if we let δ_k be a small positive value, the performance dose not. In Figure 2, we examine Method (1) in which we always choose $\delta_k = 10^{-5}$ and vary the value of t. Figure 2 shows that the parameter t hardly affects the performance of Method (1). Moreover, in Method (3), we also find that the parameter t does not have big influence on computational efficiency.

Table 3. The parameter values which give good numerical results

Method number	Values of the parameters
(1)	$t = 1, \delta_k = 10^{-5}$
(2)	$\underline{m} = 10^{-2}, \overline{M} = 10^4, l = 10^{-2}, \delta_k = 10^{-6}$
(3)	$t = 1, \xi = 10, \delta_k = 10^{-5}$

Next, we choose t=1 and compare Methods (1)-(6). For this comparison, we first changed the parameter values in the range of Table 2 except t (however, the case $\delta_k=0$ is removed), and investigated which parameter values gave good numerical results for every method. We show such values in Table 3. In Figure 3, we compare numerical performance of Methods (1)-(6) with the parameter values in Table 3. Figure 3 implies that Method (2) is the best solution, Method (3) is the second and Method (1) is the third. Hence, the msBFGS method with a suitable choice of the parameter values is superior to the standard BFGS method from the viewpoint of the CPU time. In particular, we observe that reducing the trace of B_k by Method (2) is efficient. However, Method (2) with l=1 and 10 did not perform better than the standard

BFGS method even if we suitably chose $\underline{\mathbf{m}}, \overline{M}$ and δ_k . Thus, it is preferable to select a small value for l. Furthermore, the results of Methods (1) and (3) imply that switching the scaling factor by (4.6) is efficient owing to the superliner convergence property of Method (3). In order to investigate the local behavior of Methods (1) and (3) with the parameter values in Table 3, in Figures 4 and 5, we compare the numerical results for solving the Extended Rosenbrock function (the problem 21 in [10]). These figures present the values of $\log_{10}|f_k-f_*|$, where f_* denotes the optimal value. We can find that Method (3) converges superlinearly for the Extended Rosenbrock function, but Method (1) dose not.

From the above observations, by choosing the parameter values suitably, our method performs effectively on the CPU time. Though we show the results only for the case t = 1 in Figure 3, we obtain similar results to Figure 3 for the other cases $t \in \{0, 0.25, 0.5, 0.75\}$, by selecting the parameter values suitably.

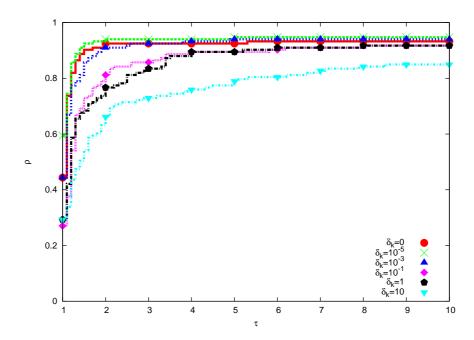


Figure 1. The case of choosing t = 1 and varying δ_k in Method (1)

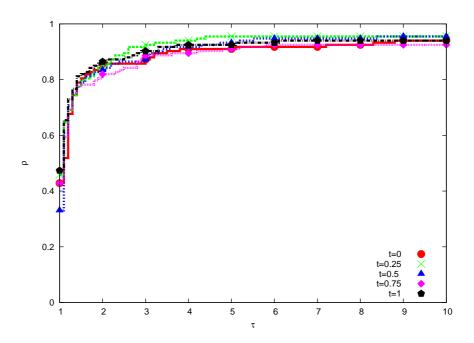


Figure 2. The case of choosing $\delta_k=10^{-5}$ and varying t in Method (1)

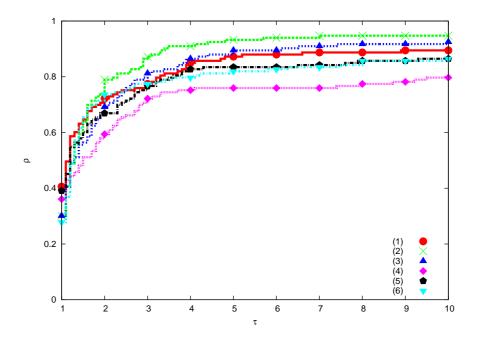


Figure 3. The comparison between Methods (1)-(6) (use the parameter values in Table 3)

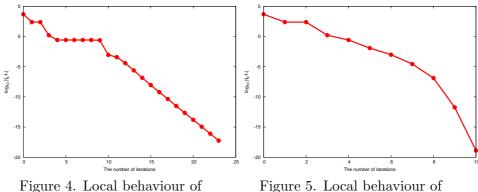


Figure 4. Local behaviour of Method (1) for Extended Rosenbrock function

Figure 5. Local behaviour of Method (3) for Extended Rosenbrock function

§6. Conclusion

In this paper, we have proposed a modified scaling BFGS method (msBFGS) for unconstrained minimization, and proved the global and superliner convergence of our method. In addition, we have applied concrete parameters (scaling factors) to the msBFGS method, proved its convergence properties and done the numerical experiments. The numerical results show that our methods perform better in general than the standard BFGS method. As further works, we would apply a scaling factor to other updating formulas.

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