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## New quasi-Newton methods via higher order tensor models

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#### ABSTRACT

Many researches attempt to improve the efficiency of the usual quasi-Newton (QN) methods by accelerating the performance of the algorithm without causing more storage demand. They aim to employ more available information from the function values and gradient to approximate the curvature of the objective function. In this paper we derive a new QN method of this type using a fourth order tensor model and show that it is superior with respect to the prior modification of Wei et al. (2006) [4]. Convergence analysis gives the local convergence property of this method and numerical results show the advantage of the modified ON method.

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### 1. Introduction

We consider the minimization of the nonlinear objective function  $f: \Re^n \to \Re$ ,

 $\min f(x)$ ,

where f is twice continuously differentiable.

The first quasi-Newton (QN) method was developed by Davidon and become one of the basic algorithms for solving nonlinear optimization. These algorithms can be viewed as a scaling on steepest descent search direction and need only the first order derivatives of the objective function. In fact they construct a convex quadratic model of the function at the current iterate  $x_k$  and measure the changes in gradients to provide information about the second derivative of f along the search direction. The model has the form of:

$$m_k(p) = f_k + g_k^T p + \frac{1}{2} p^T B_k p$$

where  $f_k$  is the value of f at  $x_k$ ,  $g_k$  denotes the gradient of f at  $x_k$  and  $B_k$  is an  $n \times n$  symmetric positive definite (SPD) matrix that approximates  $G_k$ , the Hessian matrix of f. For this model  $p_k = -B_k^{-1}g_k$  is the minimizer which allows the new iterate  $x_k = x_{k-1} + \alpha_{k-1}p_{k-1}$  where  $\alpha_{k-1}$  is the stepsize which in general is chosen to satisfy the Wolfe conditions that are given below:

$$f(x_{k-1} + \alpha_{k-1}p_{k-1}) \le f(x_{k-1}) + c_1\alpha_{k-1}g_{k-1}^T p_{k-1}$$
(1)

$$g^{T}(x_{k-1} + \alpha_{k-1}p_{k-1})p_{k-1} \ge c_2 g_{k-1}^{T} p_{k-1}. \tag{2}$$

It is required that  $m_k(p)$  and its gradient interpolate the function f and its derivatives at the two latest iterates giving the secant equation as

$$\alpha_{k-1}B_kp_{k-1} = g_k - g_{k-1}.$$

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Defining  $s_{k-1} = x_k - x_{k-1}$  and  $y_{k-1} = g_k - g_{k-1}$  simplifies the secant equation notation as

$$B_k s_{k-1} = y_{k-1}$$
.

Here if  $s_{k-1}$  and  $y_{k-1}$  satisfy the curvature condition  $s_{k-1}^T y_{k-1} > 0$  then the matrix  $B_k$  is SPD. This condition is guaranteed to hold if exact line search or Wolfe conditions have been imposed on step length  $\alpha$  (see [1]).

Other variants of QN algorithms attempt to modify these methods to upgrade their efficiency whilst maintaining important properties such as: super linear convergence, enabling them to be updated by rank two or rank one matrices, hereditary of being SPD for approximation matrices to the Hessian or inverse Hessian, requirement of cheaper arithmetic operations and invariance to transformation in the variables (see [2]). Furthermore, among all QN updating formulas, the BFGS formula possesses very effective self-correcting properties and so it is presently considered as the most effective one (see [3]).

Recently Wei [4] proposed a modified QN equation using the third order Taylor formula for the objective function given by

$$B_k s_{k-1} = \widehat{y}_{k-1}, \quad \widehat{y}_{k-1} = y_{k-1} + \frac{\psi_{k-1}}{s_{k-1}^T u} u$$

for some vector  $u \in \Re^n$  such that  $s_{k-1}^T u \neq 0$ , where

$$\psi_{k-1} = 2(f_{k-1} - f_k) + (g_k + g_{k-1})^T s_{k-1}.$$

We call the modified BFGS algorithm arising from this modified secant equation the "BFGS-type" (BFGS-T) method if the strategy used to preserve the positive definiteness of BFGS updated matrices is

$$\psi_{k-1} = (\eta - 1)s_{k-1}^T y_{k-1}, \quad \text{if } \psi_{k-1} < (\eta - 1)s_{k-1}^T y_{k-1}, \ \eta \in (0, 1).$$

Assuming that the function f is smooth enough and ||s|| is sufficiently small, then it is proved that for each vector u with  $s^T u \neq 0$ 

$$s^{T}Gs - s^{T}y = \frac{1}{2}s^{T}(Ts)s + o(\|s\|^{4})$$

$$s^{T}Gs - s^{T}\widehat{y} = \frac{1}{3}s^{T}(Ts)s + o(\|s\|^{4})$$
(3)

where T is the tensor of f at  $x_k$  and

$$s^{T}(Ts)s = \sum_{i,i,l=1}^{n} \frac{\partial^{3} f(x)}{\partial x^{i} \partial x^{j} \partial x^{l}} s^{i} s^{j} s^{l}$$

(see [4]).

In this paper, we aim to derive a new class of modified QN equations to achieve higher order accuracy in approximating the second order curvature of the objective function than the BFGS-T method does.

The paper is organized as follows. Section 2 introduces the new QN equation; the properties of this and the modified BFGS-type algorithm are presented in Section 3. Sections 4 and 5 demonstrate the convergence theory and Section 6 presents preliminary numerical results on test problems; conclusions and perspectives are finally outlined in Section 7.

## 2. Derivation of the new QN equation

In this section we derive a new QN equation which exploits both the gradients and function values and accounts for the greater curvature measured during the last step. We start the derivation of the new equation concerning the following fourth order tensor model of the objective function about the iterate  $x_k$ :

$$m_T(x_k + s) = f(x_k) + g_k \otimes s + \frac{1}{2}G_k \otimes s^2 + \frac{1}{6}T_k \otimes s^3 + \frac{1}{24}V_k \otimes s^4 + o(\|s\|^5)$$
(4)

where  $\otimes$  is an appropriate tensor product and  $V_k \in \Re^{n^4}$  is symmetric and

$$s^{T}((V_{k}s)s)s = \sum_{i,i,l,m=1}^{n} \frac{\partial^{4} f(x_{k})}{\partial x^{i} \partial x^{j} \partial x^{l} \partial x^{m}} s^{i} s^{j} s^{l} s^{m}.$$

If the model (4) interpolates the function f at  $x_{k-1}$ , we have

$$f_{k-1} = f_k - g_k \otimes s_{k-1} + \frac{1}{2} G_k \otimes s_{k-1}^2 - \frac{1}{6} T_k \otimes s_{k-1}^3 + \frac{1}{24} V_k \otimes s_{k-1}^4 + o(\|s\|^5), \tag{5}$$

differentiate (5) with respect to  $s_{k-1}$  and multiply by  $s_{k-1}$  to obtain

$$g_{k-1} \otimes s_{k-1} = g_k \otimes s_{k-1} - G_k \otimes s_{k-1}^2 + \frac{1}{2} T_k \otimes s_{k-1}^3 - \frac{1}{6} V_k \otimes s_{k-1}^4 + o(\|s\|^5).$$

After cancelling the terms involving the tensor  $V_k$  and arithmetic manipulation, we get

$$s_{k-1}^{T}G_{k}s_{k-1} = y_{k-1}^{T}s_{k-1} + \phi_{k-1} + \frac{1}{6}T_{k} \otimes s_{k-1}^{3} + o(\|s\|^{5})$$

$$(6)$$

where

$$\phi_{k-1} = 4(f_{k-1} - f_k) + 2(g_k + g_{k-1})^T s_{k-1}. \tag{7}$$

According to the equality (6), we can write the following formula:

$$s_{k-1}^{T}G_{k}s_{k-1} = s_{k-1}^{T}y_{k-1} + \phi_{k-1} + \frac{1}{6}o(\|s\|^{3}) + o(\|s\|^{5}).$$
(8)

To obtain a higher accuracy in approximating the Hessian matrix by  $B_k$ , it is reasonable to let  $B_k$  satisfy

$$s_{k-1}^T B_k s_{k-1} = s_{k-1}^T \widetilde{y}_{k-1} = s_{k-1}^T y_{k-1} + \phi_{k-1}.$$

Thus one of the possible choices in approximation of  $B_k s_{k-1}$  can be given by

$$B_k s_{k-1} = \widetilde{y}_{k-1}, \widetilde{y}_{k-1} = y_{k-1} + \frac{\phi_{k-1}}{s_{k-1}^T u} u$$
(9)

with  $s_{k-1}^T u \neq 0$  and  $u \in \Re^n$ .

The vectors  $s_{k-1}$ ,  $y_{k-1}$ ,  $-g_{k-1}$  or  $g_k$ , are some available choices to replace the vector u provided that the inner product  $s_{k-1}^T u \neq 0$ . since the choice  $u = s_{k-1}$  causes the invariant property of the QN method to not be satisfied, we prefer to choose

The replacement  $u = y_{k-1}$  implies that the QN equation can be simplified to the following form

$$B_k s_{k-1} = \widetilde{y}_{k-1}, \quad \widetilde{y}_{k-1} = \beta_{k-1} y_{k-1}$$
 (10)

where  $\beta_{k-1} = 1 + \phi_{k-1}/s_{k-1}^T y_{k-1}$ . Now quasi-Newton updating formulas can be modified when  $y_{k-1}$  is replaced by  $\widetilde{y}_{k-1}$ . So the inverse BFGS formula given

$$H_k = (I - \rho_{k-1} s_{k-1} y_{k-1}^T) H_{k-1} (I - \rho_{k-1} y_{k-1} s_{k-1}^T) + \rho_{k-1} s_{k-1} s_{k-1}^T$$

where  $\rho_{k-1} = 1/s_{k-1}^T y_{k-1}$ , is modified as follows

$$\widetilde{H}_{k} = (I - \rho_{k-1} s_{k-1} y_{k-1}^{T}) \widetilde{H}_{k-1} (I - \rho_{k-1} y_{k-1} s_{k-1}^{T}) + \frac{\rho_{k-1}}{\beta_{k-1}} s_{k-1} s_{k-1}^{T}$$

$$(11)$$

where  $\beta_{k-1}$  is given by (10).

## 3. Properties of the modified QN method and description of the new algorithm

## 3.1. Properties of the modified ON method

Most of the properties of usual QN methods are preserved for the modified version of these methods. For complete discussion see [5]. In this section we discuss the properties that are distinguishable among the usual and modified methods.

**Theorem 1.** Let the function f(x) be smooth enough. If ||s|| is sufficiently small, then for any vector u with  $s_{k-1}^T u \neq 0$  we have

$$s_{k-1}^{T}G_{k}s_{k-1} - s_{k-1}^{T}\widehat{y}_{k-1} = \frac{1}{3}T_{k}s_{k-1}^{3} + o(\|s\|^{4})$$
  
$$s_{k-1}^{T}G_{k}s_{k-1} - s_{k-1}^{T}\widetilde{y}_{k-1} = \frac{1}{6}T_{k}s_{k-1}^{3} + o(\|s\|^{5}).$$

**Proof.** See the equalities (3), (6) and (9).

Under the assumption of Theorem 1 it is intuitive that the curvatures  $s_{k-1}^T \widetilde{B} s_{k-1}$  capture the second order curvature  $s_{k-1}^T G_k s_{k-1}$  with a higher precision than the curvature  $s_{k-1}^T \widehat{B} s_{k-1}$  does.

Another property which we are concerned with here is the heredity property of positive-definite updates of QN methods. To have a descent direction and to move from one iterate to another our approximation matrices should be positive definite. This feature is maintained if we use the strategy

$$\phi_{k-1} = (\eta - 1)s_{k-1}^T y_{k-1}, \quad \text{if } \phi_{k-1} < (\eta - 1)s_{k-1}^T y_{k-1}, \ \eta \in (0, 1)$$

$$\tag{12}$$

and if exact line search or Wolfe conditions are applied to the steplength  $\alpha_{k-1}$ . The reason for this behavior is given below. The modified ON updated matrices will be positive definite if

$$s_{k-1}^{T} y_{k-1}^{\diamond} = s_{k-1}^{T} y_{k-1} + \kappa_{k-1} > 0 \tag{13}$$

where  $y_{k-1}^{\diamond}$  denotes  $\widehat{y}$  (or  $\widetilde{y}$ ) and  $\kappa$  indicates  $\psi$  (or  $\phi$ ) respectively.

The next proposition shows that near the solution, for sufficiently small  $s_k$ , the condition (13) will be satisfied.

**Proposition 2.** Suppose that the function f(x) is twice continuously differentiable. If  $\{x_k\}$  converges to a point  $x^*$  such that  $\nabla f(x*) = 0$  and  $\nabla^2 f(x*)$  is positive definite, then

$$\lim_{k \to \infty} \frac{s_{k-1}^T y_{k-1}^{\diamond}}{s_{k-1}^T y_{k-1}} = 1.$$

**Proof.** Eqs. (6) and (3) imply that  $\kappa_{k-1} = O(\|s_{k-1}\|^3)$  and  $s_{k-1}^T y_{k-1} = O(\|s_{k-1}\|^2)$  for sufficiently large k. Since  $\nabla^2 f(x^*)$  is positive definite, there exist  $\delta > 0$  such that  $s_{k-1}^T y_{k-1} \ge \delta \|s_{k-1}\|^2$  for sufficiently large k. Therefore  $\lim_{k \to \infty} \kappa_{k-1}/s_{k-1}^T y_{k-1} = 0$ , and applying this equality on Eq. (13) the conclusion follows.  $\square$ 

Therefore for general nonlinear smooth functions when the sequence  $\{x_k\}$ , produced by modified QN methods, converges to a strong local minimum point  $x^*$  of f, condition (13) holds for all sufficiently large k. For the points  $x_k$  outside the region around the local minimizer, the condition  $s_{k-1}^T y_{k-1} > 0$  is guaranteed to hold if the Wolfe (strong Wolfe) conditions hold on the line search. But for the modified QN method, from (1), (2) and (7) we have

$$s_{k-1}^{T}\widetilde{y}_{k-1} = 4(f_{k-1} - f_{k}) + g_{k-1}^{T} s_{k-1} + 3g_{k}^{T} s_{k-1}$$

$$\geq 3g_{k}^{T} s_{k-1} + (1 - 4c_{1}\alpha)g_{k-1}^{T} s_{k-1}$$

$$\geq (3c_{2} + 1 - 4c_{1})g_{k}^{T} s_{k-1}.$$
(14)

Hence we hope  $s_{k-1}^T\widetilde{y}_{k-1}>0$  if a large decrease in f is achieved and  $\|g_k^Ts_{k-1}\|$  is near to zero. To this end the values of  $c_1$  and  $c_2$  can be chosen as  $1/4< c_1<1/2$  and  $(3c_2+1-4c_1)<0$ . Also we can use the strategy (12) which gives a restriction on  $\phi_{k-1}$  and ensures  $s_{k-1}^T\widetilde{y}_{k-1}\geq \eta s_{k-1}^Ty_{k-1}>0$ .

## 3.2. Algorithm MBFGS-T

We express formally the new algorithm "Modified BFGS-type" (MBFGS-T) method as follows.

Algorithm:

Given an initial point  $x_0$ , inverse Hessian approximation  $H_0$ , convergence tolerance  $\epsilon > 0$ ;

 $k \leftarrow 1$ :

while  $\|g_{k-1}\| > \epsilon$ ;

Compute the search direction  $p_{k-1}$  by solving

$$p_{k-1} = -\widetilde{H}_{k-1}g_{k-1};$$

Choose a steplength  $\alpha_{k-1}$  along the direction  $p_{k-1}$  to satisfy the Wolfe conditions (1) and (2) and set

$$x_k = x_{k-1} + \alpha_{k-1} p_{k-1};$$

Compute  $s_{k-1} = x_k - x_{k-1}$  and  $y_{k-1} = g_k - g_{k-1}$ ;

Quantify the value of  $\phi$  via (7) and (12);

Define  $\beta_{k-1} = 1 + \phi_{k-1}/s_{k-1}^T y_{k-1}$ ;

Compute  $\widetilde{H}_k$  by means of (11);

 $k \leftarrow k + 1$ ;

end(while)

#### 4. Global convergence property

This section presents the global convergence property for the QN method with updates satisfying the modified QN equation. The global convergence result on uniformly convex functions has been proven in [6] for the BFGS method with line searches subject to the Wolfe conditions (1) and (2). In doing so, we need the following assumptions on the objective function f(x) and its gradient g(x).

**Assumption 1.** (i) The objective function f(x) is twice continuously differentiable, and for a given point  $x_0$ , the level set  $\Omega = \{x : f(x) < f(x_0)\}$  is convex.

(ii) There exist positive constants *m* and *M* such that

$$m\|z\|^2 \le z^T G z \le M\|z\|^2 \tag{15}$$

for all  $z \in \Re^n$  and  $x \in \Omega$ .

(iii) There exists a constant L > 0 such that

$$\|g(x) - g(y)\| < L\|x - y\| \quad \forall x, y \in \Omega.$$

(iv)

$$|s_{k-1}^T u| \ge \mu ||u|| \, ||s_{k-1}||, \quad \mu \in (0, 1].$$

For  $u = s_{k-1}$  the condition (iv) is satisfied with  $\mu = 1$  and for  $u = y_{k-1}$  it holds with  $\mu = \sigma_1/\sigma_2$  where  $\sigma_1$  and  $\sigma_2$  are two positive constants such that  $\sigma_1 \|v\|^2 \le v^T G(x) v \le \sigma_2 \|v\|^2$  holds for all x near  $x^*$  and any vector v in  $\Re^n$  (see [7]).

The following theorem is expressed to study the global convergence of the BFGS method satisfying conditions (1) and (2), for uniformly convex functions (see [8]).

**Theorem 3.** Suppose that the function f(x) satisfies assumptions (i)–(iii) for a given point  $x_0$  and  $B_0$  is symmetric positive definite. If the sequence  $\{x_k\}$  generated by the BFGS method with step length  $\alpha_k$  satisfying conditions (1) and (2) is not terminated at some point  $x_k$  with  $g_k = 0$ , then there exist positive constants  $a_1$ ,  $a_2$ ,  $a_3$  and  $a_4$  such that

$$\frac{\|y_k\|^2}{s_k^T y_k} \le a_1, \tag{16}$$

$$\frac{s_k^T B_k s_k}{s_k^T y_k} \le a_2 \alpha_k,\tag{17}$$

$$\frac{\|B_k s_k\|^2}{s_L^T B_k s_k} \ge a_3 \frac{\alpha_k}{\cos^2 \theta_k},\tag{18}$$

$$\frac{|y_k^T B_k s_k|}{s_k^T y_k} \le a_4 \frac{\alpha_k}{\cos \theta_k} \tag{19}$$

hold for all k and the sequence  $\{x_k\}$  converges to the unique minimizer  $x^*$  of f(x) on  $\Omega$ . Here

$$\cos \theta_k \stackrel{\text{def}}{=} \frac{s_k^T B_k s_k}{\|s_k\| \|B_k s_k\|}.$$

Based on this theorem, the global convergence result for the BFGS method can be obtained when the vector parameter  $y_k$  is replaced by  $\widetilde{y}_k$ .

**Theorem 4.** The results of Theorem 3 are satisfied if for BFGS updates  $y_k$  is replaced by  $\widetilde{y}_k$ .

**Proof.** It is enough to show that the inequalities (16)–(19) still hold for some positive constants  $a_1$ ,  $a_2$ ,  $a_3$  and  $a_4$ . Since inequality (18) depends only on  $s_k$ , we require to prove the rest of inequalities in which  $y_k$  is replaced by  $\widetilde{y}_k$ . Since

$$f_k = f_{k-1} + g_{k-1}^T s_{k-1} + \frac{1}{2} s_{k-1}^T G(x_{k-1} + t_1 s_{k-1}) s_{k-1}, \quad t_1 \in (0, 1)$$

and

$$g_k^T s_{k-1} = g_{k-1}^T s_{k-1} + \int_0^1 s_{k-1}^T G(x_{k-1} + t_2 s_{k-1}) dt s_{k-1}, \quad t_1 \in (0, 1)$$

we obtain

$$|\phi_{k-1}| = |4(f_{k-1} - f_k) + 2(g_{k-1} + g_k)^T s_{k-1}|$$

$$= |2s_{k-1}^T (-G(x_{k-1} + t_1 s_{k-1}) + \overline{G}_{k-1}) s_{k-1}| \le 4M ||s_{k-1}||^2.$$
(20)

Now from (20) and the strategy (12) the following is obtained

$$s_{k-1}^T \widetilde{y}_{k-1} \ge \eta s_{k-1}^T y \ge \eta m \|s_k\|^2,$$

and

$$\|\widetilde{y}_{k-1}\| \le \|y_{k-1}\| + \frac{|\phi_{k-1}|}{\mu \|s_{k-1}\|} \le M\left(1 + \frac{4}{\mu}\right) \|s_{k-1}\|. \tag{21}$$

Hence the inequality (16) holds with  $a_1 = M^2(1 + 4/\mu)^2/\eta m$ . From line search conditions (1) and (2), we can obtain

$$\frac{1-c_2}{M}\cos\theta_{k-1} \le \frac{\|s_{k-1}\|}{\|g_{k-1}\|} \le \frac{2(1-c_1)}{m}\cos\theta_{k-1}. \tag{22}$$

By using  $|s_{k-1}^T u| \ge \mu \|u\| \|s_{k-1}\|$  and strategy (12), it follows from (21) and (22) that

$$\frac{s_{k-1}^T B_{k-1} s_{k-1}}{s_{k-1}^T \widetilde{y}_{k-1}} \le -\frac{M \alpha_{k-1} s_{k-1}^T g_{k-1}}{m \eta (1 - c_2) (-s_{k-1}^T g_{k-1})} = \frac{M \alpha_{k-1}}{m \eta (1 - c_2)},$$

and

$$\frac{|\widetilde{y}_{k-1}^T B_{k-1} s_{k-1}|}{s_{k-1}^T \widetilde{y}_{k-1}} \le \frac{\alpha_{k-1} \|\widetilde{y}_{k-1}\| \|g_{k-1}\|}{\eta m \|s_{k-1}\|^2} \le \frac{M^2 (1 + 4/\mu) \alpha_{k-1}}{\eta m (1 - c_2) \cos \theta_{k-1}}.$$

The proof is complete.  $\Box$ 

## 5. Local convergence property

In this section local convergence results of algorithm MBFGS-T are given. For this purpose, we make the following assumptions on the objective function.

**Assumption 2.** (i) The objective function f is twice continuously differentiable on some convex set  $\Omega$  and  $x^*$  a local minimizer of f over  $\Omega$  such that  $\nabla f(x^*) = 0$  and  $G(x^*)$  is positive definite.

- (ii)  $x_0 \in \Omega$  and  $H_0$  are sufficiently close to  $x^*$  and  $G^{-1}(x^*)$ , respectively. So as mentioned before  $s_{k-1}^T \widetilde{y}_{k-1} > 0$  and  $\widetilde{y}_{k-1} = y_{k-1} + [\phi_{k-1}/s_{k-1}^T u]u$  with  $s_{k-1}^T u \neq 0$  for all k.
- (iii) The Hessian matrix G(x) is Lipschitz continuous on  $\Omega$ , that is, there exists a positive constant L such that

$$||G(x) - G(Z)|| < L||x - z|| \forall x, z \in \Omega.$$

(iv)  $|s_{k-1}^T u| \ge \mu ||u|| ||s_{k-1}||, \ \mu \in (0, 1].$ 

The local convergence result of the inverse BFGS method with steplength  $\alpha_{k-1}=1$  and

$$H_k = (I - \rho_{k-1} s_{k-1} y_{k-1}^T) H_{k-1} (I - \rho_{k-1} y_{k-1} s_{k-1}^T) + \rho_{k-1} s_{k-1} s_{k-1}^T$$
(23)

with  $\rho_{k-1} = 1/s_{k-1}^T y_{k-1}$ ,  $x_k = x_{k-1} + s_{k-1}$  and  $s_{k-1} = -H_{k-1}g_{k-1}$  is studied by the following theorem. see [9,10].

**Theorem 5.** Suppose Assumption 2 (i) holds. Let  $z_k$  be any vector which satisfies the inequalities

$$||z_{k-1} - G(x^*)s_{k-1}|| \le c(||x_k - x^*|| + ||x_{k-1} - x^*||)||s_{k-1}||$$
(24)

and

$$\frac{1}{\nu}\|s_{k-1}\| \le \|z_{k-1}\| \le \gamma \|s_{k-1}\| \tag{25}$$

for all k; where c>0 and  $\gamma>0$  are constants. Let the sequence  $\{x_k\}\subset\Omega$  be generated by the inverse BFGS method (23) with  $\alpha_k=1$ . If  $x_0$  and  $H_0$  are sufficiently close to  $x^*$  and  $G^{-1}(x^*)$ , respectively, then the bounded deterioration condition

$$||[H_k - G^{-1}(x^*)]||_M \le [\sqrt{1 - \nu \xi^2} + \nu_1 \sigma(x_{k-1}, x_k)]||H_{k-1} - G^{-1}(x^*)||_M + \nu_2 \sigma(x_{k-1}, x_k)$$

holds; the sequences  $\{\|H_k\|\}$  and  $\{\|H_k^{-1}\|\}$  are bounded; the limit

$$\lim_{k \to \infty} \|[H_{k-1} - G^{-1}(x^*)]y_{k-1}\| / \|y_{k-1}\| = 0$$

holds, and the local superlinear convergence of the sequence  $\{x_k\}$  follows; where  $\nu \in [3/8, 1], \xi \in [0, 1]\nu_1$  and  $\nu_2$  are positive constants; and  $\|A\|_M$  is the weighted matrix norm defined by  $\|A\|_M = \|MAM\|_F$  where  $\|.\|_F$  denotes the Frobenius norm and My = s.

For the normal inverse BFGS method, i.e.  $z_{k-1} = y_{k-1}$ , by the Assumption 2, (i)–(iii), (24) with c = L/2 and (25) are satisfied respectively. Thus this theorem holds for this method. According to Theorem 5, to establish the superlinear convergence of the sequence  $x_k$  generated by the MBFGS-T method, ( $z_{k-1} = \widetilde{y}_{k-1}$ ), it is required to prove some preliminary lemmas

First we consider the inverse modified BFGS formula

$$\widetilde{H}_{k} = (I - \widetilde{\rho}_{k-1} s_{k-1} \widetilde{y}_{k-1}^{T}) \widetilde{H}_{k-1} (I - \widetilde{\rho}_{k-1} \widetilde{y}_{k-1} s_{k-1}^{T}) + \widetilde{\rho}_{k-1} s_{k-1} s_{k-1}^{T}$$

$$(26)$$

with  $\widetilde{\rho}_{k-1} = 1/s_{k-1}^T \widetilde{y}_{k-1}$ ,  $x_k = x_{k-1} + s_{k-1}$  and  $s_{k-1} = -\widetilde{H}_{k-1} g_{k-1}$ .

**Lemma 6.** Suppose Assumption 2 holds. There exist  $c_1 > 0$  such that

$$\|\widetilde{y}_{k-1} - G^{-1}(x^*)s_{k-1}\| \le c_1(\|x_k - x^*\| + \|x_{k-1} - x^*\|)\|s_{k-1}\|$$
(27)

for each  $x_k, x_{k-1} \in \Omega$ .

**Proof.** We start by using the definition of  $\widetilde{y}_k$  and Assumption 2-(iv)

$$\|\widetilde{y}_{k-1} - G(x^*)s_{k-1}\| \le \|y_{k-1} - G(x^*)s_{k-1}\| + |\phi_{k-1}|/\mu \|s_{k-1}\|.$$

Since

$$f_k = f_{k-1} + g_{k-1}^T s_{k-1} + 1/2 s_{k-1}^T G(x_{k-1} + \tau s_{k-1}) s_{k-1}, \quad \tau \in (0, 1)$$

and

$$g_k^T s_{k-1} = g_{k-1}^T s_{k-1} + \int_0^1 s_{k-1}^T G(x_{k-1} + t s_{k-1}) dt s_{k-1},$$

recalling Assumption 2-(iii), we have

$$\begin{aligned} |\phi_{k-1}| &= |4(f_{k-1} - f_k) + 2(g_k + g_{k-1})^T s_{k-1}| \\ &= 2|s_{k-1}^T \int_0^1 [G(x_{k-1} + \tau s_{k-1}) - G(x_{k-1} + t s_{k-1})] dt s_{k-1}| \\ &\leq 2||s_{k-1}^T|| \int_0^1 L|\tau - t|dt ||s_{k-1}|| ||s_{k-1}|| \\ &\leq L(||x_k - x^*|| + ||x_{k-1} - x^*||)||s_{k-1}||^2. \end{aligned}$$

$$(28)$$

Hence  $|\phi_{k-1}|/\mu \|s_{k-1}\| \le 2L\sigma \|s_{k-1}\|/\mu$ . Accordingly, (27) is met by  $c_1 = (1+2/\mu)L/2$ .

**Lemma 7.** Assume that Assumption 2 holds. There exist  $\gamma_1 > 0$  such that

$$\frac{1}{\gamma_1} \|s_{k-1}\| \le \|\widetilde{y}_{k-1}\| \le \gamma_1 \|s_{k-1}\|, \quad \forall x_k, x_{k-1} \in \{x : \|x - x^*\| \le \epsilon_1\}$$
(29)

for each  $x_k, x_{k-1} \in \Omega$ .

**Proof.** From (25) with  $y_{k-1}$  replacing  $z_{k-1}$  and (28) we get

$$\begin{split} \|\widetilde{y}_{k-1}\| &\leq \|y_{k-1}\| + \frac{|\phi_{k-1}|}{\mu \|s_{k-1}\|} \leq \left[\beta + \frac{2L\sigma}{\mu}\right] \|s_{k-1}\|, \\ \|\widetilde{y}_{k-1}\| &\geq \|y_{k-1}\| - \frac{|\phi_{k-1}|}{\mu \|s_{k-1}\|} \geq \left[\frac{1}{\beta} - \frac{2L\sigma}{\mu}\right] \|s_{k-1}\|. \end{split}$$

Therefore if  $\epsilon_1 \leq \mu/2L\beta$ , then (29) holds with

$$\beta_1 = \max \left\{ \beta + \frac{2L\epsilon_1}{\mu}, \frac{\beta\mu}{\mu - 2L\beta\epsilon_1} \right\}. \quad \Box$$

**Lemma 8.** If the sequence  $\{x_k\}$  produced by (26) converges to a point  $x^*$  such that  $\|\widetilde{H}_k\|$  and  $\|\widetilde{H}_k^{-1}\|$  are bounded; then  $x_k$  converges superlinearly to  $x^*$  if

$$\lim_{k \to \infty} \frac{\|[\widetilde{H}_k - G^{-1}(x^*)]\widetilde{y}_k\|}{\|\widetilde{y}_k\|} = 0.$$

$$(30)$$

**Proof.** For the simplicity of the notation we set  $\widetilde{y}_k = y_k + \overline{y}_k$  in which  $\overline{y}_k = \frac{\phi_k}{s_k^T u} u$ . Since by (26),  $x_k = x_{k-1} - \widetilde{H}_{k-1} g_{k-1}$  we have

$$\widetilde{H}_{k-1}y_{k-1} = \widetilde{H}_{k-1}(g_k - g_{k-1}) = \widetilde{H}_{k-1}g_k + s_{k-1}.$$

Now, we can write

$$\begin{aligned} [\widetilde{H}_{k-1} - G^{-1}(x^*)]\widetilde{y}_{k-1} &= [\widetilde{H}_{k-1} - G^{-1}(x^*)](\overline{y}_{k-1} + y_{k-1}) \\ &= [\widetilde{H}_{k-1} - G^{-1}(x^*)](\overline{y}_{k-1}) + \widetilde{H}_{k-1}g_k + s_{k-1} - G^{-1}(x^*)y_{k-1}, \end{aligned}$$

which gives

$$\widetilde{H}_{k-1}g_k = [\widetilde{H}_{k-1} - G^{-1}(x^*)]\widetilde{y}_{k-1} - [\widetilde{H}_{k-1} - G^{-1}(x^*)]\overline{y}_{k-1} + G^{-1}(x^*)[y_{k-1} - G(x^*)s_{k-1}] 
= [\widetilde{H}_{k-1} - G^{-1}(x^*)]\widetilde{y}_{k-1} + G^{-1}(x^*)[\widetilde{y}_{k-1} - G(x^*)s_{k-1}] - \widetilde{H}_{k-1}\overline{y}_{k-1}.$$
(31)

Since the updated matrix and its inverse are bounded, there exist  $\vartheta_1$  and  $\vartheta_2$  such that  $\|\widetilde{H}_{k-1}\| \leq \vartheta_1$  and  $\|\widetilde{H}_{k-1}^{-1}\| \leq \vartheta_2$ . Therefore, using these relations in (31) we deduce that the following bound holds:

$$\|g_k\| \le \vartheta_2\{\|\widetilde{H}_{k-1} - G^{-1}(x^*)\widetilde{|y_{k-1}|} + \|G^{-1}(x^*)\|.\|\widetilde{y}_{k-1} - G(x^*)s_{k-1}\| + \vartheta_1\|\overline{y}_{k-1}\|\}. \tag{32}$$

Using (30) and (29) we get

$$\lim_{k \to \infty} \| [\widetilde{H}_{k-1} - G^{-1}(x^*)] \widetilde{y}_{k-1} \| / \| s_{k-1} \| = 0.$$
(33)

We have from (27)

$$\|\widetilde{y}_{k-1} - G^{-1}(x^*)s_{k-1}\|/\|s_{k-1}\| \le 2c\sigma \to 0, \quad \text{as } k \to \infty$$
 (34)

and from (28)

$$\|\overline{y}_{k-1}\|/\|s_{k-1}\| \le |\phi_{k-1}|/\mu\|s_{k-1}\|^2 \le 2L\sigma/\mu \to 0, \quad \text{as } k \to \infty.$$
 (35)

Combining (32)-(35) we obtain

$$\lim_{k \to \infty} \|g_k\| / \|s_{k-1}\| = 0. \tag{36}$$

Since by (29) we have

$$||g_k|| = ||g_k - g(x^*)|| \ge (1/\gamma_1 ||x_k - x^*||),$$

and  $||s_{k-1}|| \le 2||x_k - x^*||$ , using (36) we conclude that

$$\lim_{k\to\infty} \|x_k - x^*\| / \|x_{k-1} - x^*\| = 0. \quad \Box$$

With these three lemmas the local superlinear convergence of the MBFGS-T algorithm indicated by (26) with  $\alpha_{k-1} = 1$  can be expressed as follows.

**Theorem 9.** Suppose that Assumption 2 holds. If  $x_0 \in \Omega$  and  $\widetilde{H}_0$  are sufficiently close to  $x^*$  and  $G^{-1}(x^*)$ ; respectively, then the sequence  $x_k$  generated by the MBFGS-T method ( $\alpha_k = 1$  for all k) converges superlinearly to  $x^*$ .

#### 6. Numerical results

This section describes some numerical results on the test problems selected from collection [11] implemented in the PC machine. The codes are written in Fortran 77 in double precision, including BFGS, BFGS-T and MBFGS-T algorithms for which the algorithm 500 [12] is utilized. A line search routine is used based on cubic interpolation that satisfies the Wolfe conditions (1) and (2), with  $c_1 = 0.01$  and  $c_2 = 0.9$  and all the runs reported in this section terminate when

$$f_{k-1} - f_k \le 10^{-8} \max\{1.0, |f_{k-1}|\} \text{ or } ||g|| \le 10^{-4} \max\{1.0, ||x_{k-1}||\}.$$

Forty six test problems as listed in Table 1 are examined with standard starting points. The identity matrix has been chosen as an initial inverse matrix. Ten different dimensions between 4 and 1000 are chosen and the maximum number of function and gradient evaluations is set at 2000.

To get positive definite updates, the strategy (12) with  $\eta = 10^{-4}$  is employed for both modified methods.

Based on the performance profiles [13] The fraction P of problems is plotted, for which any given method is within a factor  $\tau$  of the best time.

**Table 1**Selected test problems for BFGS and modified methods.

Extended Freudenstein and Roth – Dixmaane (CUTE) – Quadratic QF1 – Diagonal 3 – Extended Tridiagonal 2 – Extended Penalty – Vardim (CUTE) – Extended EP1 – Generalized Tridiagonal 1 – Dixon3dq (CUTE) – Raydan 2 – Partial Perturbed Quadratic PPQ2 – Extended Tridiagonal 1 – Perturbed Quadratic – Tridia (CUTE) – Extended Rosenbrock – Bdqrtic (CUTE) – Diagonal 5 – Extended Quadratic Penalty QP1 – Generalized PSC1 – NONDQUAR (CUTE) – Biggsb1 (CUTE) – Extended Maratos – Quadratic QF2 – Scaled Quadratic SQ1 – Dqdrtic (CUTE) – Extended Beale – Generalized Tridiagonal 2 – Arwhead (CUTE) – FLETCHCR (CUTE) – Extended Himmelblau – Dixmaana (CUTE) – Diagonal 4 – Partial Perturbed Quadratic PPQ1 – Broyden Tridiagonal Perturbed Quadratic – Edensch (CUTE) – Diagonal 1 – Staircase S1 – Liarwhd (CUTE) – Diagonal 6 – SINQUAD (CUTE) – Dixmaani (CUTE) – Extended White and Holst – Extended Three Expo Terms

**Table 2**Relative efficiency of BFGS method, algorithms BFGS-T, MBFGS-T in arithmetic means.

	Iteration	FG call	Time
BFGS-T	0.9788	0.9785	0.9307
MBFGS-T	0.9409	0.9512	0.8865

**Table 3**Relative efficiency of BFGS-T method, algorithm MBFGS-T in arithmetic means.

	Iteration	FG call	Time
MBFGS-T	0.9607	0.9718	0.9547

**Table 4**Relative efficiency of BFGS method, algorithms BFGS-T and MBFGS-T in geometric means.

	Iteration	FG call	Time
BFGS-T	0.9787	0.979	0.9006
MBFGS-T	0.9366	0.9502	0.8483

**Table 5**Relative efficiency of BFGS-T method, algorithm MBFGS-T in geometric means.

	Iteration	FG call	Time
MBFGS-T	0.957	0.9705	0.942

Further numerical experiments are conducted to show how useful the new modified algorithms are in performance. The performance profiles ideas of Dolan and More [13] can be used with another two measures, number of iterations and number of function and gradient evaluations.

These algorithms are also compared with the help of arithmetic and geometric means of three methods as given in Tables 2–5 respectively.

From the Figs. 1–3, MBFGS-T is always the top performer for most values of  $\tau$ . Table 2 shows that for the arithmetic mean over BFGS, MBFGS-T is 0.038 faster than BFGS-T in number of iterations, 0.0273 faster in number of functions and gradient evaluations and 0.0442 faster in time. Also for the geometric mean as seen in Table 4, over BFGS, MBFGS-T is 0.0421 faster than BFGS-T in number of iterations, 0.0289 faster in number of function and gradient evaluations and 0.0522 faster in time. In addition Tables 3 and 5, indicate the advantage of the MBFGS-T method in comparison with the BFGS-T method.

The storage and arithmetics are the same for the modified BFGS algorithms dicussed in this paper and they are insignificant compared to BFGS. Furthermore a higher order accuracy in approximating the inverse Hessian matrix of the objective function occurs for the new method. Hence it is concluded that MBFGS-T performs better than the BFGS-T and BFGS methods and improves the performance, requiring fewer iterations, fewer function and gradient evaluations and less time.

#### 7. Conclusion

A new QN equation is proposed using the fourth order tensor model of the objective function. The modified equation can reduce the multiplier of the third order error term to 1/6 and drop the fourth order error term as well make a better approximation to the Hessian matrix than the prior modification of Wei et al. [4] does. Theoretically, the algorithms involving the QN equation such as those mentioned in [14], using this new modification can be upgraded in efficiency by reduction

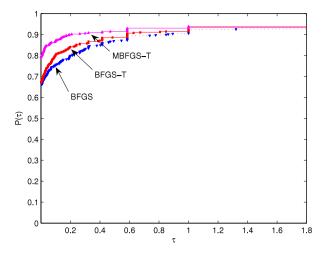


Fig. 1. Performance profiles based on time.

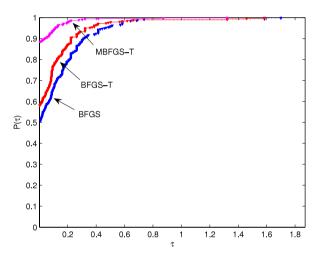


Fig. 2. Performance profiles based on number of iterations.

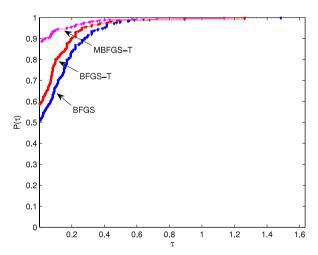


Fig. 3. Performance profiles based on function/gradient calls.

in number of iterations and function and gradient calls and time. Experience in the frame of the BFGS algorithm shows that the MBFGS-T outperforms the BFGS and BFGS-T algorithms.

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