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A New Sparse Quasi-Newton Update Method

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ABSTRACT: Based on the idea of maximum determinant positive definite matrix completion, Yamashita proposed a sparse quasi-Newton update, called MCQN, for unconstrained optimization problems with sparse Hessian structures. Such an MCQN update keeps the sparsity structure of the Hessian while relaxing the secant condition. In this paper, we propose an alternative to the MCQN update, in which the quasi-Newton matrix satisfies the secant condition, but does not have the same sparsity structure as the Hessian in general. Our numerical results demonstrate the usefulness of the new MCQN update with the BFGS formula for a collection of test problems. A local and superlinear convergence analysis is also provided for the new MCQN update with the DFP formula.

KEYWORDS: Large-scale, Matrix completion, Quasi-Newton methods, Secant condition, Sparsity, Unconstrained optimization.

تحسين جديد لطريقة متماثلة نيوتن المتناثرة

منغو تشينج و يوهونج داي و روي دياو

ملخص: بالاستناد إلى فكرة إكمال المحدد الأقصى لمصفوفة موجبة محددة، اقترح ياماشيتا تحسيناً لطريقة متماثلة نيوتن المتناثرة وسماها MCQN وذلك لحل مسائل الأمثليات غير المقيدة مع أصفار متناثرة في مصفوفة هس. يحافظ هذا التحسين على هيكلية التناثر في مصفوفة هس مع تخفيف شرط القاطع. نقترح في هذا البحث بديلا عن تحسين MCQN بحيث تكون مصفوفة متماثلة نيوتن محققة لشرط القاطع، ولكنها لاتمتلك نفس هيكلية التناثر لمصفوفة هس بشكل عام. تبين نتائجنا العددية فائدة استخدام تحسين MCQN الجديد مع قانون BFGS لحل مجموعة من المسائل التجريبية. كذلك تم تحليل التقارب الموضعي والخطي الفائق لتحسين قانون MCQN الجديد مع قانون DFP.

1. Introduction

Consider the unconstrained optimization problem

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

where $f : R^n \to R$ is continuously differentiable and its gradient $\nabla f(x)$ is available. If the dimension n is not large, the quasi-Newton method is one choice for solving problem (1) because of its superlinear convergence and the unnecessity to calculate the function Hessian. Assuming that x_k is the current iterate and H_k is the approximation to the inverse Hessian, the quasi-Newton method generates the next iterate by

$$x_{k+1} = x_k - \alpha_k H_k \nabla f(x_k), \tag{2}$$

where $\alpha_k > 0$ is a stepsize obtained via some line search, and updates the approximation H_k to H_{k+1} to meet the secant condition

$$H_{k+1} y_k = s_k, \tag{3}$$

where $s_k = x_{k+1} - x_k$ and $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$.

If the dimension of the problem (1) is large, the direct use of the quasi-Newton method is not possible due to the storage of an $n \times n$ matrix. In order to overcome this difficulty, several methods have been proposed. The limited-memory BFGS (L-BFGS) method (Liu and Nocedal, 1989; Nocedal, 1980) is only to store a few curvature pairs (s_i, y_i) in the construction of the Hessian approximation. Since there is no need to know any information about the Hessian, the L-BFGS method is friendly to users and has been widely used in practice. For many large-scale problems, the function f can be written in the form

$$f(x) = \sum_{i=1}^{n_e} f_i(x),$$

where each of the n_e element functions f_i depends only on a few variables. In this case, the partitioned quasi-Newton method, developed by Griewank and Toint (see Griewank and Toint, 1982a, 1982b; Griewank and Toint, 1984; and the references therein), performs very well in practice, and is now regarded as one of the important practical optimization algorithms. Their basic idea is to update a Hessian approximation B_k^i for each element function f_i and then to assemble these matrices to obtain an approximation B_k to the whole Hessian of *f*. Further, they determine the search direction by solving the linear system

$$\left(\sum_{i=1}^{n_e} B_k^i\right) d_k = -\nabla f(x_k).$$

Their method was implemented with the trust region strategy since the matrix B_k is not positive definite in general.

There are also many large-scale problems where the function Hessian $\nabla^2 f(x)$ is sparse and the sparsity structure is available. Suppose that for all $x \in R^n$,

$$[\nabla^2 f(x)]_{i,j} = 0, \quad (i,j) \in F, \tag{4}$$

where F is some subset of $I \times I$ and $I = \{1, 2, \cdots, n\}$. In this case, it is possible to establish faster optimization methods by exploiting the sparsity structure of the Hessian. Toint (1977) and Fletcher (1995) studied such updates and required H_{k+1} to meet the sparsity requirement, namely, $(H_{k+1}^{-1})_{i,j} = (B_{k+1})_{i,j} = 0$ when $(i,j) \in F$, and the secant equation (3) simultaneously. As a result, their methods involve the solution of a linear system or a convex program at each iteration. If some component of s_k is zero, the obtained approximate Hessian may be ill-posed (see Sorensen's example (Sorensen, 1982)). Inspired by the successful use of positive definite matrix completion in (Fukuda *et al.*, 2000) for semidefinite programming, Yamashita (2008) proposed a novel type of quasi-Newton update for problem (1) satisfying the sparse Hessian structure. Let $\psi : R^{n \times n} \to R$ be a strictly convex function defined by

$$\psi(A) = \mathrm{tr}(A) - \ln\det(A) \tag{5}$$

(This function is introduced in (Byrd and Nocedal, 1989) as a powerful tool for the convergence analysis of quasi-Newton methods). Yamashita determines the new approximation matrix H_{k+1} from H_k by two steps:

(i) update H_k to H^{QN} by certain ordinary quasi-Newton formula;

(ii) obtain H_{k+1} by solving the following subproblem with H,

$$\begin{aligned} \min \quad & \psi(H_k^{-1/2} H H_k^{-1/2}) \\ \text{s.t.} \quad & H_{i,j} = H_{i,j}^{QN}, \quad (i,j) \in F \\ & (H^{-1})_{i,j} = 0, \quad (i,j) \notin F \\ & H \in S_+ . \end{aligned} \tag{6}$$

Here S_+ denotes the set of symmetric positive semidefinite matrices. Notice that since step (ii) uses $H_{i,j}^{QN}$, $(i,j) \in F$, we only have to update $|F|$ elements of H_k in step (i), where $|F|$ means the cardinality of F. As in (Yamashita, 2008), we call the above update MCQN (Matrix Completion Quasi-Newton). The use of DFP and BFGS methods in step (i) are considered in (Yamashita, 2008).

Further, Yamashita showed that, if the sparsity pattern of the Hessian is such that there is not any fill-in in its Cholesky factorization, or equivalently, the graph induced by the Hessian is chordal (see (Yamashita, 2008) for details), problem (6) is equivalent to finding a maximum-determinant positive definite matrix completion of $H_{i,j}^{QN}$, $(i,j) \in F$:

$$\begin{aligned} \max \quad & \det(H) \\ \text{s.t.} \quad & H_{i,j} = H_{i,j}^{QN}, \quad (i,j) \in F \\ & H \in S_+ . \end{aligned} \tag{7}$$

The above problem can be easily solved by analyzing the clique tree of the graph induced by the Hessian (see (Yamashita, 2008) for details). In addition, it is shown in (Yamashita, 2008) that the update does not suffer from the drawback in Sorensen's example (Sorensen, 1982). Therefore by relaxing the secant equation, the MCQN update is easy to implement and is well-posed.

The numerical experiments in (Yamashita, 2008) show that, the MCQN update with BFGS obviously performs better than the MCQN update with DFP. As seen from the above procedure, the MCQN update by Yamashita keeps the sparsity structure of the Hessian, but does not satisfy the quasi-Newton condition. Nevertheless, local and superlinear convergence results are only established for an MCQN update with DFP. Dai and Yamashita (2007) extended the results to the MCQN update with Broyden's family.

In this paper, we propose an alternative of the MCQN update, in which the quasi-Newton matrix satisfies the secant condition, but does not have the same sparsity structure as the Hessian in general (see the next section). A local and superlinear convergence analysis is also provided for the new MCQN update with DFP (see Section 3). Our numerical results for a collection of test problems demonstrate that the new MCQN update with BFGS clearly outperforms the previous MCQN update with BFGS (see Section 4). Conclusions and discussions are presented in the last section.

2. The new MCQN method

Looking back to the MCQN update by Yamashita (2008), the whole sequence of quasi-Newton matrices, which were used for the calculations of search directions, keep the same sparsity structure as the function Hessian. The intermediate matrix H^{QN} satisfies the secant condition, but does not necessarily have the same sparsity structure as the function Hessian. As an alternative of such an MCQN update, we may think of the possible use of those intermediate matrices in the calculations of search directions. In this paper, we explore this possibility and our numerical results in Section 4 demonstrate the usefulness of such an idea.

To describe the new MCQN update, we assume that the current quasi-Newton matrix is H_k, which is symmetric and positive definite. Since H_k does not have the sparsity structure of the function Hessian in general, we consider the optimal solution of the following subproblem as an intermediate matrix H_k^S,

$$\begin{aligned} \min \quad & \psi(H_k^{-1/2} H H_k^{-1/2}) \\ \text{s.t.} \quad & H_{i,j} = (H_k)_{i,j}, \quad (i,j) \in F \\ & (H^{-1})_{i,j} = 0, \quad (i,j) \notin F \\ & H \in S_+, \end{aligned} \tag{8}$$

where, again S_+ denotes the set of symmetric positive semidefinite matrices and F is some subset of $I \times I$ such that (4) holds. If the graph induced by the Hessian is chordal (otherwise, we extend the set F such that the induced graph has such property), we know that H_k^S possesses the sparse structure and has the following form of sparse clique factorization

$$H = P_1^T P_2^T \cdots P_l^T Q P_l P_{l-1} \cdots P_2 P_1, \tag{9}$$

where $P_i, i = 1, 2, \cdots, l$ and Q are some sparse matrices (see (Yamashita, 2008)). Having obtained the intermediate matrix H_k^S, we can use for example the BFGS formula to generate a new quasi-Newton matrix

$$H_{k+1} = H_k^S - \frac{H_k^S y_k s_k^T + s_k y_k^T H_k^S}{s_k^T y_k} + \left(1 + \frac{y_k^T H_k^S y_k}{s_k^T y_k}\right) \frac{s_k s_k^T}{s_k^T y_k}, \tag{10}$$

which satisfies the secant condition $H_{k+1} y_k = s_k$ and will be used for the calculation of search directions. In other words, we alter the two steps in the original MCQN method and determine the new approximation matrix H_{k+1} in the following way:

(i) obtain H_k^S by solving problem (7);

(ii) update H_k^S to H_{k+1} by certain quasi-Newton formula.

It is not difficult to see that the amount of computation of such a strategy is almost the same as that required by the original MCQN. However, since the new approximation matrix H_{k+1} satisfies exactly the secant condition, we think that the new quasi-Newton matrix H_{k+1} contains more information about the function Hessian. The numerical results confirm our idea.

A description of the new sparse quasi-Newton method is given as follows.

Algorithm 2.1 *(NMCQN)*

Step 1. Obtain an extension of F (still denoted by F) such that $G(V, F)$ is chordal. Choose $x_0 \in R^n$ and a positive definite matrix H_0 with $(H_0^{-1})_{ij} = 0, \forall (i,j) \notin F$. Set $k := 0$.

Step 2. If x_k satisfies the termination criterion, then stop.

Step 3. $x_{k+1} = x_k - H_k \nabla f(x_k)$.

Step 4. Obtain the sparse clique-factorization formula (9) of H_k^S.

Step 5. Obtain H_{k+1}, $(i,j) \in F$ by some ordinary quasi-Newton update.

Step 6. Set $k := k + 1$ and go to Step 2.

We call the New MCQN method NMCQN. If, in Step 5, the quasi-Newton matrix H_{k+1} is obtained from H_k^S by (10), we denote $H_{k+1} = \mathrm{BFGS}(H_k^S, s_k, y_k)$ and call the corresponding algorithm NMCQN-BFGS. If the DFP update formula is used, namely,

$$H_{k+1} = H_k^S - \frac{H_k^S y_k y_k^T H_k^S}{y_k^T H_k^S y_k} + \frac{s_k s_k^T}{s_k^T y_k}, \tag{11}$$

we denote $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$ and call the corresponding algorithm NMCQN-DFP.

3. Convergence analysis

In this section, we show the local and superlinear convergence of NMCQN-DFP, namely, Algorithm 2.1 with $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$. The results are established in a manner similar to (Yamashita, 2008).

We give the following assumptions on the objective function, where $\|\cdot\|$ means the two-norm.

Assumption 3.1 Let x_* be a solution of (1) and let $\mathcal{C} = \{x \in R^n : \|x - x_*\| \le b\}$ with a positive constant *b*.

(i) The objective function *f* is twice continuously differentiable on $\mathcal{C}$.

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

$$m\|z\|^2 \le z^T \left(\nabla^2 f(x)\right)^{-1} z \le M\|z\|^2, \quad \forall z \in R^n$$

for all $x \in \mathcal{C}$.

If the second-order sufficient optimality condition holds at the solution x_* and *b* is sufficiently small, Assumption 3.1(ii) holds. From Assumption 3.1(i), $\nabla^2 f(x)$ is Lipschitz continuous on $\mathcal{C}$. Then, from Lemmas 4.1.12 and 4.1.15 in (Dennis and Schnabel, 1983), there exist L_1 and L_2 such that for all $x_k, x_{k+1} \in \mathcal{C}$,

$$\left\|y_k - \nabla^2 f(x_*) s_k\right\| \le L_1 \|s_k\|^2 \tag{12}$$

and

$$\left\|y_k - \nabla^2 f(x_*) s_k\right\| \le L_2 \varepsilon_k \|s_k\|, \tag{13}$$

where ε_k is defined by

$$\varepsilon_k = \max\left\{\|x_{k+1} - x_*\|, \|x_k - x_*\|\right\}. \tag{14}$$

Moreover, there exists a positive constant L_3 such that for all $z_1, z_2 \in \mathcal{C}$,

$$\|\nabla f(z_1) - \nabla f(z_2)\| \le L_3 \|z_1 - z_2\|. \tag{15}$$

Therefore, we have

$$\|y_k\| = \|\nabla f(x_{k+1}) - \nabla f(x_k)\| \le L_3 \|s_k\| \quad \forall x_k, x_{k+1} \in C. \tag{16}$$

From Eq. (8.1.2) of (Nocedal and Wright, 1999) we have

$$y_k = \bar{G}_k s_k, \tag{17}$$

where $\bar{G}_k$ is the average Hessian defined by $\bar{G}_k = \int_0^1 \nabla^2 f(x_k + t s_k)\, dt$.

For convenience, the following notations are used in the analysis.

$$G_* = \nabla^2 f(x_*), \quad H_* = \left[\nabla^2 f(x_*)\right]^{-1}, \quad \tilde{s}_k = H_*^{-1/2} s_k, \quad \tilde{y}_k = H_*^{1/2} y_k,$$

$$\tilde{H}_k^S = H_*^{-1/2} H_k^S H_*^{-1/2}, \quad \tilde{H}_k = H_*^{-1/2} H_k H_*^{-1/2},$$

$$\cos\tilde{\theta}_k = \frac{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k}{\|\tilde{y}_k\| \|\tilde{H}_k^S \tilde{y}_k\|}, \quad \tilde{q}_k = \frac{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k}{\|\tilde{y}_k\|^2}, \qquad \tilde{M}_k = \frac{\|\tilde{s}_k\|^2}{\tilde{y}_k^T \tilde{s}_k}, \quad \tilde{m}_k = \frac{\tilde{y}_k^T \tilde{s}_k}{\tilde{y}_k^T \tilde{y}_k},$$

where $\tilde{\theta}_k$ is the angle between $\tilde{y}_k$ and $\tilde{H}_k \tilde{y}_k$.

Firstly, we introduce the following two lemmas similarly to (Yamashita, 2008).

Lemma 3.1 Suppose that Assumption 3.1 holds. Then there exist $c \in (0,\infty)$ and $\gamma \in (0,b)$ such that

$$\ln \tilde{m}_k \ge -2c\varepsilon_k,$$
$$\tilde{M}_k \le 1 + c\varepsilon_k.$$

whenever $\varepsilon_k < \gamma$.

Lemma 3.2 Suppose that Assumption 3.1 holds. Consider Algorithm 2.1 with $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$. Then we have

$$\psi(\tilde{H}_k^S) \le \psi(\tilde{H}_k),$$

where $\psi(A) = \mathrm{tr}(A) - \ln\det(A)$.

By using the above lemmas, we show the following key inequality.

Lemma 3.3 Suppose that Assumption 3.1 holds. Consider Algorithm 2.1 with $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$. Let γ be the constant specified in (13). If $\varepsilon_k \le \gamma$, then we have

$$\psi(\tilde{H}_{k+1}) + \ln\frac{1}{\cos^2\tilde{\theta}_k} - \left[1 - \frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k} + \ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right] \le \psi(\tilde{H}_k) + 3c\varepsilon_k.$$

Proof. By Assumption 3.1(ii) and (17), we have

$$\frac{y_k^T s_k}{y_k^T y_k} = \frac{y_k^T \bar{H}_k y_k}{y_k^T y_k} \ge m$$

and

$$\frac{y_k^T y_k}{y_k^T s_k} = \frac{z_k^T \bar{H}_k z_k}{z_k^T z_k} \le M,$$

where $z_k = \bar{H}_k^{-1/2} y_k$ and $\bar{H}_k = \bar{G}_k^{-1}$.

Since H_{k+1} is obtained from H_k^S by the DFP formula, we have

$$\begin{aligned}
\tilde{H}_{k+1} &= H_*^{-1/2} H_{k+1} H_*^{-1/2} \\
&= H_*^{-1/2} H_k^S H_*^{-1/2} - H_*^{-1/2}\left(\frac{H_k^S y_k y_k^T H_k^S}{y_k^T H_k^S y_k} - \frac{s_k s_k^T}{y_k^T s_k}\right) H_*^{-1/2} \\
&= \tilde{H}_k^S - \frac{\tilde{H}_k^S H_*^{1/2} y_k y_k^T H_*^{1/2} \tilde{H}_k^S}{y_k^T H_*^{1/2} H_*^{-1/2} H_k^S H_*^{-1/2} H_*^{1/2} y_k} + \frac{H_*^{-1/2} s_k s_k^T H_*^{-1/2}}{y_k^T H_*^{1/2} H_*^{-1/2} s_k}
\end{aligned}$$

$$= \tilde{H}_k^S - \frac{\tilde{H}_k^S \tilde{y}_k \tilde{y}_k^T \tilde{H}_k^S}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k} + \frac{\tilde{s}_k \tilde{s}_k^T}{\tilde{y}_k^T \tilde{s}_k}. \tag{18}$$

Since $\mathrm{tr}(zz^T) = \|z\|^2$ for $z \in R^n$, it follows from (18) that

$$\mathrm{tr}(\tilde{H}_{k+1}) = \mathrm{tr}(\tilde{H}_k^S) - \frac{\left\|\tilde{H}_k^S \tilde{y}_k\right\|^2}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k} + \frac{\|\tilde{s}_k\|^2}{\tilde{y}_k^T \tilde{s}_k}. \tag{19}$$

In a manner similar to the use of Eqs. (8.45) in (Nocedal and Wright, 1999), we can show that

$$\det(\tilde{H}_{k+1}) = \det(\tilde{H}_k^S) \frac{\tilde{y}_k^T \tilde{s}_k}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k}. \tag{20}$$

Moreover, simple calculations show that

$$\frac{\tilde{y}_k^T \tilde{s}_k}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k} = \frac{\tilde{y}_k^T \tilde{s}_k}{\|\tilde{y}_k\|^2} \frac{\|\tilde{y}_k\|^2}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k} = \frac{\tilde{m}_k}{\tilde{q}_k} \tag{21}$$

and

$$\frac{\left\|\tilde{H}_k^S \tilde{y}_k\right\|^2}{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k} = \frac{\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k}{\|\tilde{y}_k\|^2} \frac{\left\|\tilde{H}_k^S \tilde{y}_k\right\|^2 \|\tilde{y}_k\|^2}{(\tilde{y}_k^T \tilde{H}_k^S \tilde{y}_k)^2} = \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k}. \tag{22}$$

It follows from (19), (20), (21) and (22) that

$$\begin{aligned} \psi(\tilde{H}_{k+1}) &= \mathrm{tr}(\tilde{H}_{k+1}) - \ln\det(\tilde{H}_{k+1}) \\ &= \mathrm{tr}(\tilde{H}_k^S) + \tilde{M}_k - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} - \ln\det(\tilde{H}_k^S) - \ln \tilde{m}_k + \ln \tilde{q}_k \\ &= \psi(\tilde{H}_k^S) + \tilde{M}_k - \ln \tilde{m}_k - 1 + 1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \cos^2 \tilde{\theta}_k . \end{aligned} \tag{23}$$

Lemmas 3.2 and 3.3 give

$$\tilde{M}_k - \ln \tilde{m}_k - 1 \le 1 + c\varepsilon_k + 2c\varepsilon_k - 1 = 3c\varepsilon_k$$

and

$$\psi(\tilde{H}_k^S) \le \psi(\tilde{H}_k).$$

Then it follows from (23) that

$$\psi(\tilde{H}_{k+1}) \le \psi(\tilde{H}_k) + 3c\varepsilon_k + \ln \cos^2 \tilde{\theta}_k + 1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k}. \tag{24}$$

Therefore

$$\psi(\tilde{H}_{k+1}) + \ln \frac{1}{\cos^2 \tilde{\theta}_k} - \left[1 - \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k} + \ln \frac{\tilde{q}_k}{\cos^2 \tilde{\theta}_k}\right] \le \psi(\tilde{H}_k) + 3c\varepsilon_k , \tag{25}$$

which completes the proof. □

Using inequality (25), the local and superlinear convergence will be shown.

Theorem 3.1 Suppose that Assumption 3.1 holds. Consider Algorithm 2.1 with $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$. Then, for any $\alpha \in (0,1)$, there exist τ_x and τ_H such that $\|x_0 - x_*\| \le \tau_x$ and $\|H_0 - H_*\| \le \tau_H$ imply

$$\|x_{k+1} - x_*\| \le \alpha \|x_k - x_*\|, \text{ for all } k.$$

Proof. Suppose that $\alpha \in (0,1)$. The following inequalities will be shown to hold for all *k*,

$$\|x_{k+1} - x_*\| \le \alpha \|x_k - x_*\|, \tag{26}$$

$$\|H_k - H_*\| \le \frac{\alpha}{2L_3}, \tag{27}$$

where L_3 is the Lipschitz constant of ∇f.

First, note that by choosing τ_x to be sufficiently small, we have

$$L_1 M \tau_x < \frac{\delta}{2}, \quad \tau_x \le \gamma, \tag{28}$$

where L_1, M and γ are the constants specified in (12), Assumption 3.1(ii) and (13), respectively. Moreover, according to Lemma 4 in (Yamashita, 2008), by choosing τ_x and τ_H to be sufficiently small, there exists $\delta \in (0, \alpha)$ such that

$$\psi(\tilde{H}_0) - n < \frac{\delta}{2}, \tag{29}$$

$$\psi(\tilde{H}) - n < \delta \quad \Rightarrow \quad \|H - H_*\| \le \frac{\alpha}{2L_3} \tag{30}$$

and

$$\frac{3c\tau_x}{1-\alpha} \le \frac{\delta}{2}, \tag{31}$$

where *H* is a symmetric positive definite matrix, $\tilde{H} = H_*^{-1/2} H H_*^{-1/2}$, and *c* is the constant specified in Lemma 3.1.

We prove the theorem by induction. When $k = 0$, the inequality (27) holds from (29) and (30). Moreover, we have

$$\begin{aligned}
\|x_1 - x_*\| &= \|x_0 - H_0 \nabla f(x_0) - x_*\| \\
&\le \|x_0 - x_* - H_* \nabla f(x_0)\| + \|(H_0 - H_*)(\nabla f(x_0) - \nabla f(x_*))\| \\
&\le \|H_*(\nabla f(x_0) - \nabla f(x_*) - G_*(x_0 - x_*))\| + L_3 \|H_0 - H_*\| \|x_0 - x_*\| \\
&\le L_1 \|H_*\| \|x_0 - x_*\|^2 + \frac{\alpha}{2} \|x_0 - x_*\| \\
&\le (L_1 M \tau_x + \frac{\alpha}{2}) \|x_0 - x_*\| \\
&\le \alpha \|x_0 - x_*\|.
\end{aligned}$$

where the second inequality follows from (15), the third inequality follows from (12) and (30), the forth inequality follows from Assumption 3.1(ii) and $\|x_0 - x_*\| \le \tau_x$, and the final inequality follows from (28) and $\delta < \alpha$.

Next, assuming (26) and (27) for $k = 0, 1, \cdots, l-1$, we shall show they are also true for $k = l$. In fact, similarly to the case in which $k = 0$, we have

$$\begin{aligned}\|x_{l+1}-x_*\| &= \|x_l - H_l\nabla f(x_l)-x_*\| \\ &\le \|x_l - x_* - H_*\nabla f(x_l)\| + \|(H_l - H_*)(\nabla f(x_l)-\nabla f(x_*))\| \\ &\le \|H_*(\nabla f(x_l)-\nabla f(x_*)-G_*(x_l-x_*))\| + L_3\|H_l - H_*\|\|x_l - x_*\| \\ &\le L_1\|H_*\|\|x_l - x_*\|^2 + \frac{\alpha}{2}\|x_l - x_*\| \\ &\le (L_1 M\|x_l - x_*\| + \frac{\alpha}{2})\|x_l - x_*\|\end{aligned}$$

and thus

$$\begin{aligned}\|x_{l+1}-x_*\| &\le (L_1 M\alpha^l\tau_x + \frac{\alpha}{2})\|x_l - x_*\| \\ &\le \alpha\|x_l - x_*\|\end{aligned}$$

where the first inequality follows from the induction assumption. This shows the truth of (26) for $k=l$. In the following, we show (27) by (25) in Lemma 3.3. Summing up the inequality (25) with $k=0,1,\cdots,l-1,$ we have

$$\psi(\tilde{H}_l)+\sum_{k=0}^{l-1}\left(\ln\frac{1}{\cos^2\tilde{\theta}_k}-\left[1-\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}+\ln\frac{\tilde{q}_k}{\cos^2\tilde{\theta}_k}\right]\right)\le\psi(\tilde{H}_0)+3c\sum_{k=0}^{l-1}\varepsilon_k .$$

Since $0<\cos\tilde{\theta}_k\le 1$ and the term in the square brackets is nonpositive, we have

$$\psi(\tilde{H}_l)-n\le\psi(\tilde{H}_0)-n+3c\sum_{k=0}^{l-1}\varepsilon_k . \tag{32}$$

From (14) and the induction assumption, we have

$$\varepsilon_k = \max\left\{\|x_{k+1}-x_*\|,\|x_k - x_*\|\right\}\le\max\left\{\alpha^{k+1}\tau_x,\alpha^k\tau_x\right\}=\alpha^k\tau_x$$

for $k=0,1,\cdots,l-1,$ and thus

$$\sum_{k=0}^{l-1}\varepsilon_k \le \sum_{k=0}^{l-1}\alpha^k\tau_x = \frac{1-\alpha^l}{1-\alpha}\tau_x \le \frac{\tau_x}{1-\alpha}.$$

It then follows from (32), (29) and (31) that

$$\psi(\tilde{H}_l)-n\le\psi(\tilde{H}_0)-n+\frac{3c\tau_x}{1-\alpha}<\delta .$$

From (30), we have $\|H_l-\nabla^2 f(x_*)^{-1}\|\le\frac{\alpha}{2L_3},$ which is (27) for $k=l$. Thus by induction, (26) and (27) hold for all k. □

In order to show the superlinear convergence, we build the following relationship similarly to (Yamashita, 2008),

$$\lim_{k\to\infty}\frac{\|(H_k - H_*)y_k\|}{\|y_k\|}=0 \quad\Rightarrow\quad \lim_{k\to\infty}\frac{\|(B_k - G_*)s_k\|}{\|s_k\|}=0. \tag{33}$$

Lemma 3.4 Suppose that Assumption 3.1 holds. Consider Algorithm 2.1 with $H_{k+1}=\mathrm{DFP}(H_k^S,s_k,y_k)$. Suppose also that $\|x_0 - x_*\|\le\tau_x$ and $\|H_0 - H_*\|\le\tau_H$ with the constants τ_x and τ_H specified in Theorem 3.1 for sufficiently small $\alpha\in(0,1)$. Then relationship (33) holds.

Proof. Let $\lambda_i^k, i = 1, 2, \cdots, n$ be the eigenvalues of H_k. Since the inequality (27) holds for sufficiently small α, we can assume that there exists $\lambda_{min} > 0$ such that $\lambda_i^k \geq \lambda_{min}$ for all i and k. Moreover, since $y_k = G_* s_k + (\bar{G}_k - G_*) s_k$, we have

$$\begin{aligned} \|(H_k - H_*) y_k\| &= \|(H_k - H_*) G_* s_k + (H_k - H_*)(\bar{G}_k - G_*) s_k\| \\ &\geq \|H_k (G_* - B_k) s_k\| - \|H_k - H_*\| \|\bar{G}_k - G_*\| \|s_k\| \\ &\geq \lambda_{min} \|(B_k - G_*) s_k\| - \|H_k - H_*\| \|\bar{G}_k - G_*\| \|s_k\|. \end{aligned}$$

It then follows from (16) that

$$\frac{\|(H_k - H_*) y_k\|}{\|y_k\|} \geq \frac{\lambda_{min} \|(B_k - G_*) s_k\|}{L_3 \|s_k\|} - \frac{\|(H_k - H_*)\| \|\bar{G}_k - G_*\|}{L_3}.$$

Since $\bar{G}_k = \int_0^1 \nabla^2 f(x_k + t s_k)\, dt$ and $x_k \to x_*$ by Theorem 3.1, the second term of the right-hand side of the inequality converges to 0 as $k \to \infty$. Then, relationship (33) holds. □

In the following, we give the main result of this section.

Theorem 3.2 Suppose that Assumption 3.1 holds. Suppose also that $\|x_0 - x_*\| \leq \tau_x$ and $\|H_0 - H_*\| \leq \tau_H$ hold for sufficiently small $\tau_x, \tau_H > 0$. Then the sequence $\{x_k\}$ generated by Algorithm 2.1 with $H_{k+1} = \mathrm{DFP}(H_k^S, s_k, y_k)$ converges to x_* superlinearly.

Proof. From Lemma 3.4, it suffices to show

$$\lim_{k \to \infty} \frac{\|(H_k - H_*) y_k\|}{\|y_k\|} = 0. \tag{34}$$

Notice by Theorem 3.1 that for any $\alpha \in (0,1)$, relation (27) holds provided $\tau_x, \tau_H > 0$ are sufficiently small. Then we must have that

$$\lim_{k \to \infty} \|H_k - H_*\| = 0, \tag{35}$$

otherwise there is a contradiction. Therefore (34) is true since $\|(H_k - H_*) y_k\| \leq \|H_k - H_*\| \|y_k\|$. By Lemma 3.4, we conclude the superlinear convergence of the algorithm. □

Comparing the proof of Theorem 4 in (Yamashita, 2008), the above proof is simpler and is directly obtained by one statement in Theorem 3.1.

4. Numerical results

We tested the new MCQN algorithm with the DFP and BFGS formulas, namely, NMCQN-DFP and NMCQN-BFGS, by using Matlab R2008a on Core(TM)2 PC with Windows-XP. We used the three problems in (Yamashita, 2008) and two more problems in (Dai and Yamashita, 2007) in our numerical experiments. Various dimensions, namely, $n = 10$, 100, 1000 and 10000, were chosen for the problems. All tested problems were tridiagonal. Therefore, the chordal extensions of their sparsity pattern can easily be obtained.

The details of the problems are given as follows, where x_{ini} means the used initial point.

Problem I (TRIDIA (Gould and Toint, 2003))

$$f(x) = (x_1 - 1)^2 + \sum_{i=2}^{n} (x_{i-1} - 2x_i)^2,$$

$$x_{ini} = (1, 1, \cdots, 1)^T.$$

Problem II (Extended Rosenbrock function (Fletcher,1995))

$$f(x) = \sum_{i=1}^{n-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i)^2,$$

$$x_{ini} = (-1.2, 1, -1.2, 1, \cdots, -1.2, 1)^T.$$

Problem III (Boundary value problem (Fletcher,1995))

$$f(x) = \frac{1}{2} x^T T x - e_n^T x - \frac{1}{(n+1)^2} \sum_{i=1}^{n} (\cos x_i + 2x_i),$$

$$x_{ini} = (\frac{1}{n+1}, \frac{2}{n+1}, \cdots, \frac{n}{n+1})^T,$$

where $e_n = (1, 1, \cdots, 1)^T$,

$$T = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{pmatrix}.$$

Problem IV (Extended Powell singular function (Moré *et al*., 1981))

$$f(x) = \sum_{i=1}^{n/4} \left[10(x_{4i-3} - x_{4i})^4 + (x_{4i-2} - 2x_{4i-1})^4 + 5(x_{4i-1} - x_{4i})^2 + (x_{4i-3} + 10x_{4i-2})^2 \right],$$

$$x_{ini} = (3, -1, 0, 1, \cdots, 3, -1, 0, 1)^T.$$

Problem V (Broyden tridiagonal function (Moré *et al*., 1981))

$$\begin{aligned} f(x) = \; & (3x_1 - 2x_1^2 - 2x_2 + 1)^2 + (3x_n - 2x_n^2 - x_{n-1} + 1)^2 \\ & + \sum_{i=2}^{n-1} (3x_i - 2x_i^2 - x_{i-1} - 2x_{i+1} + 1)^2, \end{aligned}$$

$$x_{ini} = (-1, \cdots, -1)^T.$$

The following termination criterion is employed:

$$\frac{\|\nabla f(x_k)\|}{n} \le 10^{-5} \quad \text{or} \quad k > 50000.$$

Instead of Step 3 in Algorithm 2.1, we set $x_{k+1} = x_k - \alpha_k H_k \nabla f(x_k)$ with a step size α_k to improve the numerical performance. α_k is chosen to satisfy Wolfe's rule :

$$f(x_k + \alpha_k d_k) - f(x_k) \leq 10^{-4} \alpha_k \nabla f(x_k)^T d_k,$$
$$|\nabla f(x_k + \alpha_k d_k)^T d_k| \leq -0.9 \nabla f(x_k)^T d_k.$$

For convenience, we also list the numerical results reported for the MCQN update, as well as for the BFGS and L-BFGS methods, in (Yamashita, 2008). See Tables 1 and 2. For the L-BFGS method, $m = 5$, which is the number of stored curvature pairs of L-BFGS, and the scaling factor $s_{k-1}^T y_{k-1} / \|y_{k-1}\|^2$ was employed. L-BFGS just stores the pairs of vectors $(s_k, y_k), k = 1, \cdots, m$, while our method just stores a few entries of H_k to exploit the sparsity structure of the Hessian. Therefore, both of them have fast implementation in practice.

Although NMCQN-DFP has a nice theoretical convergence property as shown in the previous section, its numerical performance is not very good. Hence we only list the results of NMCQN-BFGS. The tables list the total number of iterations. The symbol "F" denotes that the number of iterations exceeds 50000 and "-" means that the BFGS method could not be implemented for $n = 10000$.

Table 1. Results of problems I, II and III

Problem	n	BFGS	L-BFGS	MCQN-DFP	MCQN-BFGS	NMCQN-BFGS
I	10	15	31	20	29	47
	100	108	126	167	72	75
	1000	662	415	1498	192	195
	10000	-	1191	11626	528	475
II	10	78	68	76	60	514
	100	487	527	665	341	1002
	1000	4525	4979	6574	3207	690
	10000	-	49580	F	31737	403
III	10	15	24	15	15	13
	100	107	299	49	50	18
	1000	571	3117	86	54	23
	10000	-	F	2600	402	25

Table 2. Results for problems IV and V

Problem	n	MCQN-BFGS	NMCQN-BFGS
IV	10	40	37
	100	211	324
	1000	589	121
	10000	998	97
V	10	30	52
	100	56	54
	1000	49	61
	10000	56	52

The results in Table 1 show that NMCQN-BFGS is the best among the methods compared. For Problems IV and V, we only present numerical results for MCQN-BFGS by Yamashita (2008) and NMCQN-BFGS. From Tables 1 and 2, we can see that the NMCQN-BFGS method performs much better than MCQN-BFGS and BFGS and L-BFGS.

For a further comparison between NMCQN-BFGS with MCQN-BFGS, we tested the new method with different choices of initial points. The initial points for the five test problems are x_{ini}, $2x_{ini}$, $4x_{ini}$, $7x_{ini}$ and $10x_{ini}$. The dimension of the test problems are fixed to be $n = 1000$. We list the number of iterations of the two methods for different test problems in Table 3. The results show that NMCQN-BFGS is better than MCQN-BFGS. Therefore the new method, NMCQN-BFGS, is a promising alternative of MCQN-BFGS especially for large-scale problems.

5. Conclusions and discussion

In this paper, we have proposed an alternative to the sparse quasi-Newton update method (MCQN) by Yamashita (2008). The quasi-Newton matrix in the new MCQN method (denoted by NMCQN) satisfies exactly the secant condition, but does not possess the same sparsity structure as the function Hessian in general. We have established the local and superlinear convergence of NMCQN with the DFP updating formula, namely, NMCQN-DFP. The numerical experiments showed that NMCQN-BFGS is promising especially for large-scale problems.

Table 3. Results with different initial points

Problem	Initial Point	MCQN-BFGS	NMCQN-BFGS	Problem	Initial Point	MCQN-BFGS	NMCQN-BFGS
I	x_{ini}	192	195	IV	x_{ini}	54	121
	$2x_{ini}$	210	202		$2x_{ini}$	213	191
	$4x_{ini}$	213	199		$4x_{ini}$	210	249
	$7x_{ini}$	220	215		$7x_{ini}$	228	370
	$10x_{ini}$	213	210		$10x_{ini}$	294	252
II	x_{ini}	3207	690	V	x_{ini}	54	61
	$2x_{ini}$	4850	3753		$2x_{ini}$	213	54
	$4x_{ini}$	5056	3786		$4x_{ini}$	210	90
	$7x_{ini}$	2157	813		$7x_{ini}$	228	130
	$10x_{ini}$	4961	853		$10x_{ini}$	294	62
III	x_{ini}	54	23				
	$2x_{ini}$	213	24				
	$4x_{ini}$	210	24				
	$7x_{ini}$	228	24				
	$10x_{ini}$	294	25				

It still remains under investigations how to provide a good combination of the MCQN update and the new NMCQN method by adaptively choosing one of them based on the property of the problems. When the sparsity dominates the performance, the MCQN update may be preferable; otherwise we could implement the NMCQN update. In addition, the new update method can obviously be extended to the whole Broyden's convex family.

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