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Symmetric rank-one method based on some modified secant conditions for unconstrained optimization

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Abstract. The symmetric rank-one (SR1) method is one of the well-known quasi-Newton methods, and many researchers have studied the SR1 method. On the other hand, to accelerate quasi-Newton methods, some researchers have proposed variants of the secant condition. In this paper, we propose SR1 methods based on some modified secant conditions. We analyze local behaviors of the methods. In order to establish the global convergence of the methods, we apply the trust region method to our methods.

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§1. Introduction

We consider the following unconstrained minimization problem:

$$\text{minimize} \quad f(x), \qquad f : \boldsymbol{R}^n \to \boldsymbol{R}, \qquad x \in \boldsymbol{R}^n \tag{1.1}$$

where f is sufficiently smooth and its gradient g and Hessian H are available. Quasi-Newton methods for solving (1.1) are iterative methods of the form:

$$x_{k+1} = x_k + s_k. \tag{1.2}$$

In quasi-Newton methods, the step s_k is generated based on an approximation to the Hessian $H(x_k)$, say B_k. Most of quasi-Newton methods generate B_k which satisfies the secant condition:

$$B_{k+1} s_k = y_k, \tag{1.3}$$

where $y_k = g(x_k + s_k) - g_k$ and $g_k = g(x_k)$. There are some updating formulas for B_k that include the BFGS update, the DFP update and the symmetric rank-one (SR1) update, for instance.

We do not specify how to compute s_k in (1.2). If we use a line search technique, then s_k is defined by $s_k = -\alpha_k B_k^{-1} g_k$, where $\alpha_k > 0$ is an appropriate stepsize. On the other hand, if we use a trust region technique, then s_k is an approximate solution of the following subproblem:

$$\min_{s \in R^n} \quad g_k^T s + \frac{1}{2} s^T B_k s \qquad \text{subject to} \quad \|s\| \leq \Delta_k,$$

where $\Delta_k > 0$ is a trust region radius. In trust region techniques, s_k is not always a "step" but is only an "approximate solution", and hence we set $x_{k+1} = x_k$ if s_k is not appropriate as a step. Thus we should note that (1.2) is not necessarily satisfied in trust region approaches.

The SR1 update formula is defined by

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

where $r_k = y_k - B_k s_k$. Many researchers have studied the SR1 method. For example, Conn et al. [2] showed that the approximate matrix B_k based on the SR1 update converges to the Hessian at the solution. Khalfan et al. [7] proved the R-superlinear convergence of the SR1 method under mild assumptions. Byrd et al. [1] proposed a quasi-Newton method with the SR1 update based on the trust region technique. There are many other studies on SR1 methods which include [8, 9, 11, 14, 15, 17].

On the other hand, to accelerate quasi-Newton methods, some researchers have proposed variants of the secant condition (1.3) including [5, 10, 16, 18, 19]. In this paper, we treat SR1 update formula based on some modified secant conditions, and analyze local behaviors of quasi-Newton methods based on those SR1 update formulas.

This paper is organized as follows. In Section 2, we state some modified secant conditions and give SR1 update formulas based on these modified secant conditions. In Section 3, we analyze local behaviors of the SR1 methods given in Section 2. In Section 4, in order to establish the global convergence of the methods, we apply the trust region method to the SR1 methods described in Section 2. Finally, in Section 5, preliminary numerical results are given.

In this paper, we use the symbol $\|\cdot\|$ to denote the usual ℓ_2-norm of a vector or the corresponding induced matrix norm.

§2. SR1 update formulas based on modified secant conditions

In this section, we consider SR1 update formulas based on some modified secant conditions. To this end, we briefly review those modified secant conditions.

Zhang et al. [18, 19] set the equation:

$$s_k^T B_{k+1} s_k = s_k^T y_k + \theta_k,$$

where

$$\theta_k = 6(f(x_k) - f(x_k + s_k)) + 3(g_k + g(x_k + s_k))^T s_k.$$

Based on the above equation, Zhang et al. gave a modified secant condition:

$$B_{k+1} s_k = z_k, \qquad z_k = y_k + \frac{\theta_k}{s_k^T u_k} u_k, \tag{2.1}$$

where $u_k \in \boldsymbol{R}^n$ is any vector such that $s_k^T u_k \neq 0$. If $\|s_k\|$ is sufficiently small, then we have, for any vector u_k satisfying $s_k^T u_k \neq 0$, that

$$s_k^T (H(x_k + s_k)s_k - y_k) = O(\|s_k\|^3),$$
$$s_k^T (H(x_k + s_k)s_k - z_k) = O(\|s_k\|^4).$$

It follows from these relations that the curvature $s_k^T B_{k+1} s_k$ given by any quasi-Newton update with condition (2.1) approximates the second-order curvature $s_k^T H(x_k + s_k) s_k$ with a higher precision than the curvature $s_k^T B_{k+1} s_k$ with the condition (1.3) does.

Wei et al. [16] consider another equation:

$$s_k^T B_{k+1} s_k = s_k^T y_k + \eta_k,$$

where

$$\eta_k = 2(f(x_k) - f(x_k + s_k)) + (g_k + g(x_k + s_k))^T s_k. \tag{2.2}$$

Based on the above equation, Wei et al. gave another modified secant condition:

$$B_{k+1} s_k = z_k, \qquad z_k = y_k + \frac{\eta_k}{s_k^T u_k} u_k, \tag{2.3}$$

where $u_k \in \boldsymbol{R}^n$ is any vector such that $s_k^T u_k \neq 0$. Note that the approximation matrix based on the above secant condition satisfies the following relation:

$$f(x_k) = f(x_k + s_k) + g(x_k + s_k)^T (-s_k) + \frac{1}{2}(-s_k)^T B_{k+1} (-s_k).$$

Now we estimate z_k in secant conditions (2.1) and (2.3). To this end, we give the following assumption and lemma.

Assumption.

A1. The objective function f is twice continuously differentiable everywhere, and the Hessian H is Lipschitz continuous, that is, there exists a constant L such that

$$\|H(x) - H(y)\| \leq L\|x - y\|$$

for all $x,\ y \in \boldsymbol{R}^n$.

Lemma 2.1. *Assume that Assumption* A1 *holds and there exists a positive constant γ such that $|s_k^T u_k| \geq \gamma \|s_k\| \|u_k\| > 0$ for all k. Then*

$$\left\| \frac{\eta_k}{s_k^T u_k} u_k \right\| \leq \frac{L}{\gamma} \|s_k\|^2$$

holds for any k.

Proof. We first note that $g(x_k + s_k) = g_k + \int_0^1 H(x_k + ts_k)s_k\ dt$. Then, from (2.2) and the mean value theorem, we have, for all k,

$$\begin{aligned}
|\eta_k| &= |2(f(x_k) - f(x_k + s_k)) + (g_k + g(x_k + s_k))^T s_k| \\
&= \left| 2(-g_k^T s_k - \frac{1}{2} s_k^T H(x_k + \xi s_k) s_k) + (2 g_k^T s_k + \int_0^1 s_k^T H(x_k + ts_k) s_k\ dt) \right| \\
&= \left| \int_0^1 s_k^T (H(x_k + ts_k) - H(x_k + \xi s_k)) s_k\ dt \right| \\
&\leq \|s_k\|^2 \int_0^1 \|H(x_k + ts_k) - H(x_k + \xi s_k)\|\ dt \\
&\leq L\|s_k\|^2 \int_0^1 \|(x_k + ts_k) - (x_k + \xi s_k)\|\ dt \\
&= L\|s_k\|^3 \int_0^1 |t - \xi|\ dt \\
&\leq L\|s_k\|^3,
\end{aligned}$$

where $\xi \in (0,1)$, the second inequality follows from the Lipschitz continuity of H, and the last inequality from $|t - \xi| \leq 1$. Since we have from $|s_k^T u_k| \geq \gamma \|s_k\| \|u_k\|$ that $\|u_k\| / |s_k^T u_k| \leq 1/(\gamma \|s_k\|)$, the proof is complete. □

Let x_* be a local solution of (1.1) and, for any $i \leq j$, define

$$\varepsilon_{i,j} = \max\{\|x_t - x_*\|,\ \|x_t + s_t - x_*\| \mid i \leq t \leq j\}.$$

Then we have $\|s_k\| \leq \|x_k + s_k - x_*\| + \|x_k - x_*\| \leq 2\varepsilon_{k,k}$. Hence, by Lemma 2.1, z_k in (2.3) can be estimated by

$$z_k = y_k + \frac{\eta_k}{s_k^T u_k} u_k = y_k + O(\|s_k\|^2) = y_k + O(\varepsilon_{k,k} \|s_k\|). \tag{2.4}$$

From the relation $\theta_k = 3\eta_k$, z_k in (2.1) also can be estimated by

$$z_k = y_k + \frac{\theta_k}{s_k^T u_k} u_k = y_k + O(\varepsilon_{k,k}\|s_k\|). \tag{2.5}$$

Li and Fukushima [10] proposed the following Levenberg-Marquardt type secant condition:

$$B_{k+1}s_k = z_k, \qquad z_k = y_k + \nu_k s_k, \tag{2.6}$$

where ν_k is a positive parameter such that $\nu_k = O(\|g_k\|)$ or $O(1)$. By choosing ν_k appropriately, $z_k^T s_k > 0$ can be ensured. Li and Fukushima show the global convergence of the BFGS method based on (2.6) for nonconvex unconstrained optimization problems. We assume, in this paper, $\nu_k = O(\|g_k\|)$ to establish a fast rate of convergence of our modified SR1 method. Then we can estimate z_k in (2.6) by

$$z_k = y_k + \nu_k s_k = y_k + O(\|g_k\|\|s_k\|) = y_k + O(\varepsilon_{k,k}\|s_k\|), \tag{2.7}$$

where the last equality follows from the relation $\|g_k\| = \|g_k - g(x_*)\|$ and the Lipschitz continuity of g.

From estimates (2.4), (2.5) and (2.7), we can treat secant conditions (2.1), (2.3) and (2.6) as members of the following unified secant condition:

$$B_{k+1}s_k = z_k, \qquad z_k = y_k + q_k, \tag{2.8}$$

where q_k is a vector such that

$$\|q_k\| \leq \tau\varepsilon_{k,k}\|s_k\|, \tag{2.9}$$

and τ is a nonnegative constant. Based on the modified secant condition (2.8), we will construct the modified SR1 update formula:

$$B_{k+1} = B_k + \frac{\widehat{r}_k \widehat{r}_k^T}{\widehat{r}_k^T s_k}, \tag{2.10}$$

where $\widehat{r}_k = z_k - B_k s_k$. In the paper, we consider the method which uses (2.10) and $z_k = y_k + q_k$ with (2.9), and call this method MRS1 (Modified SR1).

§3. Local behavior of MSR1

In this section, we investigate the local behavior of MSR1. We now make assumptions on the approximate matrices B_k and the sequence of iterates generated by the MSR1.

Assumption.

A2. There exists a positive constant c_1 *such that*

$$|\widehat{r}_k^T s_k| \geq c_1 \|\widehat{r}_k\| \|s_k\| > 0 \tag{3.1}$$

holds for all k.

A3. The sequence $\{x_k\}$ *converges to a local solution* x_*.

A4. The sequence $\{s_k\}$ *is uniformly linearly independent, that is, there exist a positive constant* c_2 *and positive integers* k_0 *and* m *such that, for all* $k \geq k_0$*, one can choose* n *distinct indices*

$$k \leq k_1 < \cdots < k_n \leq k + m$$

with

$$\sigma_{min}(S_k) \geq c_2,$$

where $\sigma_{min}(S_k)$ *is the minimum singular value of the matrix*

$$S_k = \left(\frac{s_{k_1}}{\|s_{k_1}\|}, \cdots, \frac{s_{k_n}}{\|s_{k_n}\|} \right).$$

We need the condition (3.1) in the convergence analysis of MSR1. On the other hand, if the condition (3.1) does not hold and if $|\widehat{r}_k^T s_k|$ is very small, then we have $z_k^T s_k \approx s_k^T B_k s_k$. Hence in actual computations, we can use B_k instead of B_{k+1} if (3.1) does not hold.

We define here the matrix

$$\widehat{H}_\ell = \int_0^1 H(x_\ell + t s_\ell) dt \tag{3.2}$$

for each ℓ. Recall that the relation $y_\ell = \widehat{H}_\ell s_\ell$ holds, which will be used in the sequel. In order to investigate the rate of convergence of the MSR1, we give the following useful lemma (see also [2, Lemma 1] and [7, Lemma 3.1]).

Lemma 3.1. *Assume that Assumptions* A1 *and* A2 *hold. Let* $\{x_k\}$ *be a sequence generated by the MSR1. Then the following statements hold*:

$$\|z_j - B_{j+1} s_j\| = 0 \tag{3.3}$$

for all j *and*

$$\|z_j - B_i s_j\| \leq \frac{2}{c_1}(L + \tau) \left(1 + \frac{2}{c_1}\right)^{i-j-2} \varepsilon_{j,i-1} \|s_j\| \tag{3.4}$$

for all j *and* $i \geq j + 1$.

Proof. We first see that (3.3) and (3.4) with $i = j+1$ immediately result from (2.8). Next, we show (3.4) by using induction on i. We choose $k \ge j+1$ and assume that (3.4) holds for all $i = j+1, \dots, k$. It follows from (2.8) and (2.9) that, for $k \ge j+1$,

$$\begin{aligned} |z_k^T s_j - s_k^T z_j| &\le |y_k^T s_j - s_k^T y_j| + |q_k^T s_j - s_k^T q_j| \\ &\le |y_k^T s_j - s_k^T y_j| + \|q_k\|\|s_j\| + \|s_k\|\|q_j\| \\ &\le |y_k^T s_j - s_k^T y_j| + \tau\varepsilon_{k,k}\|s_k\|\|s_j\| + \tau\varepsilon_{j,j}\|s_k\|\|s_j\| \\ &\le |y_k^T s_j - s_k^T y_j| + 2\tau\varepsilon_{j,k}\|s_k\|\|s_j\|, \end{aligned}$$

where the last inequality used $\varepsilon_{j,j},\ \varepsilon_{k,k} \le \varepsilon_{j,k}$. Thus from the induction assumption, we have that, for $k \ge j+2$,

$$\begin{aligned} |\widehat{r}_k^T s_j| &= |z_k^T s_j - s_k^T B_k s_j| \\ &\le |z_k^T s_j - s_k^T z_j| + |s_k^T (z_j - B_k s_j)| \\ &\le |y_k^T s_j - s_k^T y_j| + 2\tau\varepsilon_{j,k}\|s_k\|\|s_j\| \\ &\quad + \frac{2}{c_1}(L+\tau)\left(1 + \frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k-1}\|s_k\|\|s_j\|, \end{aligned} \tag{3.5}$$

while we have from (3.3) that, for $k = j+1$,

$$\begin{aligned} |\widehat{r}_{j+1}^T s_j| &= |z_{j+1}^T s_j - s_{j+1}^T B_{j+1} s_j| \\ &= |z_{j+1}^T s_j - s_{j+1}^T z_j| \\ &\le |y_{j+1}^T s_j - s_{j+1}^T y_j| + 2\tau\varepsilon_{j,j+1}\|s_{j+1}\|\|s_j\|. \end{aligned} \tag{3.6}$$

Next note from the relation $y_\ell = \widehat{H}_\ell s_\ell$ that we obtain

$$|y_k^T s_j - s_k^T y_j| = |s_k^T(\widehat{H}_k - \widehat{H}_j)s_j| \le \|\widehat{H}_k - \widehat{H}_j\|\|s_k\|\|s_j\|.$$

Since it follows from the Lipschitz continuity of H that

$$\begin{aligned} \|\widehat{H}_k - \widehat{H}_j\| &= \left\| \int_0^1 (H(x_k + ts_k) - H(x_j + ts_j))dt \right\| \\ &\le \int_0^1 \|H(x_k + ts_k) - H(x_j + ts_j)\|dt \\ &\le L \int_0^1 \|x_k + ts_k - x_j - ts_j\|dt \\ &\le L \int_0^1 (t\|x_k + s_k - x_*\| + (1-t)\|x_k - x_*\|)\ dt \\ &\quad + L \int_0^1 (t\|x_j + s_j - x_*\| + (1-t)\|x_j - x_*\|)\ dt \\ &\le L\varepsilon_{k,k} + L\varepsilon_{j,j} \\ &\le 2L\varepsilon_{j,k}, \end{aligned}$$

where the third inequality comes from $x_k + ts_k - x_* = t(x_k + s_k - x_*) + (1 - t)(x_k - x_*)$, we get

$$|y_k^T s_j - s_k^T y_j| \le 2L\varepsilon_{j,k}\|s_k\|\|s_j\|.$$

Then, for $k \ge j+2$, (3.5) yields

$$(3.7) \qquad \begin{aligned} |\widehat{r}_k^T s_j| &\le 2(L+\tau)\varepsilon_{j,k}\|s_k\|\|s_j\| \\ &\quad + \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k-1}\|s_k\|\|s_j\|, \end{aligned}$$

while we have from (3.6) that, for $k = j+1$,

$$(3.8) \qquad |\widehat{r}_{j+1}^T s_j| \le 2(L+\tau)\varepsilon_{j,j+1}\|s_{j+1}\|\|s_j\|.$$

It follows from (2.10), (3.1) and (3.7) that, for $k \ge j+2$,

$$\begin{aligned} \|z_j - B_{k+1}s_j\| &= \left\| z_j - B_k s_j - \frac{\widehat{r}_k \widehat{r}_k^T s_j}{\widehat{r}_k^T s_k} \right\| \\ &\le \|z_j - B_k s_j\| + \frac{|\widehat{r}_k^T s_j|}{c_1\|s_k\|} \\ &\le \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k-1}\|s_j\| + \frac{2}{c_1}(L+\tau)\varepsilon_{j,k}\|s_j\| \\ &\quad + \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k-1}\|s_j\| \\ &= \frac{4}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k-1}\|s_j\| + \frac{2}{c_1}(L+\tau)\varepsilon_{j,k}\|s_j\|. \end{aligned}$$

Since $c_1 \in (0,\ 1)$ and $k \ge j+2$ yield $1 \le (1+2/c_1)^{k-j-2}$ and $3 < 1 + 2/c_1$, and since $\varepsilon_{j,k-1} \le \varepsilon_{j,k}$, we have, for $k \ge j+2$, that

$$\begin{aligned} \|z_j - B_{k+1}s_j\| &\le \frac{4}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k}\|s_j\| \\ &\quad + \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k}\|s_j\| \\ &= \frac{6}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-2} \varepsilon_{j,k}\|s_j\| \\ &\le \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k-j-1} \varepsilon_{j,k}\|s_j\|. \end{aligned}$$

Similarly, we have from (2.10), (3.1), (3.3) and (3.8) that, for $k = j + 1$,

$$\begin{aligned} \|z_j - B_{j+2}s_j\| &\le \left\| z_j - B_{j+1}s_j - \frac{\widehat{r}_{j+1}\widehat{r}_{j+1}^T s_j}{\widehat{r}_{j+1}^T s_{j+1}} \right\| \\ &= \frac{\|\widehat{r}_{j+1}\| \, |\widehat{r}_{j+1}^T s_j|}{|\widehat{r}_{j+1}^T s_{j+1}|} \\ &\le \frac{|\widehat{r}_{j+1}^T s_j|}{c_1\|s_{j+1}\|} \\ &\le \frac{2}{c_1}(L+\tau)\varepsilon_{j,j+1}\|s_j\|. \end{aligned}$$

These inequalities give (3.4) for $i = k + 1$ where $k \ge j + 1$, and therefore (3.4) follows. □

By using Lemma 3.1, we have the next theorem.

Theorem 3.1. *Assume that Assumptions* A1–A4 *hold. Let* $\{x_k\}$ *be a sequence generated by the MSR1. Then there exists a positive constant* c_3 *such that, for all* $k \ge k_0$,

$$\|B_{k+m+1} - H(x_*)\| \le c_3\varepsilon_{k,k+m}, \tag{3.9}$$

where k_0 *and* m *are positive integers given in Assumption* A4. *Moreover, we have*

$$\lim_{k\to\infty} \|B_k - H(x_*)\| = 0. \tag{3.10}$$

Proof. Since we have, from (3.2) and the Lipschitz continuity of H, that

$$\begin{aligned} \|\widehat{H}_j - H(x_*)\| &\le L\int_0^1 \|x_j + ts_j - x_*\| \, dt \\ &\le L\int_0^1 (t\|x_j + s_j - x_*\| + (1-t)\|x_j - x_*\|) \, dt \\ &\le L\varepsilon_{j,j} \end{aligned}$$

holds for all $j \ge 1$, it follows from (2.8) and $y_j = \widehat{H}_j s_j$ that

$$\begin{aligned} \|z_j - H(x_*)s_j\| &= \|(\widehat{H}_j - H(x_*))s_j + q_j\| \\ &\le \|\widehat{H}_j - H(x_*)\|\|s_j\| + \|q_j\| \\ &\le L\varepsilon_{k,k+m}\|s_j\| + \tau\varepsilon_{k,k+m}\|s_j\| \\ &= M_1\varepsilon_{k,k+m}\|s_j\| \end{aligned} \tag{3.11}$$

for any $j \in \{k, k+1, \ldots, k+m\}$, where $M_1 = L+\tau$, and the second inequality used (2.9) and $\varepsilon_{j,j} \le \varepsilon_{k,k+m}$. Moreover, since $(k+m+1)-j-2 < m$ for any such j, we have from (3.4) that

$$\|z_j - B_{k+m+1}s_j\| \le \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^m \varepsilon_{k,k+m}\|s_j\| = M_2\varepsilon_{k,k+m}\|s_j\|, \tag{3.12}$$

where $M_2 = \frac{2}{c_1}(L+\tau)(1+2/c_1)^m$. By (3.11) and (3.12), we obtain, for any $j \in \{k, \ldots, k+m\}$, that

$$\frac{\|(B_{k+m+1} - H(x_*))s_j\|}{\|s_j\|} \le \frac{\|z_j - H(x_*)s_j\|}{\|s_j\|} + \frac{\|z_j - B_{k+m+1}s_j\|}{\|s_j\|} \le (M_1+M_2)\varepsilon_{k,k+m}. \tag{3.13}$$

Since (3.13) holds for any $j \in \{k_1, \ldots, k_n\}$ (recall Assumption A4), we have

$$\begin{aligned} \|B_{k+m+1} - H(x_*)\| &\le \frac{1}{c_2}\|(B_{k+m+1} - H(x_*))S_k\| \\ &\le \frac{\sqrt{n}}{c_2}\max_{j=k_1,\ldots,k_n}\left\|(B_{k+m+1} - H(x_*))\frac{s_j}{\|s_j\|}\right\| \\ &\le \frac{\sqrt{n}}{c_2}(M_1+M_2)\varepsilon_{k,k+m}, \end{aligned} \tag{3.14}$$

where the first inequality follows from $\|A\| \le \|AS_k\|\|S_k^{-1}\|$ and $\|S_k^{-1}\| = 1/\sigma_{min}(S_k) \le 1/c_2$ by Assumption A4, the second inequality from

$$\|A\| \le \sqrt{\sum_{j=1}^{n}\|a_j\|^2} \le \sqrt{n}\max_{1\le j\le n}\|a_j\|,$$

where a_j denotes the jth column of A, and the last inequality from (3.13). The relation (3.14) implies (3.9) with $c_3 = \sqrt{n}(M_1+M_2)/c_2$. Now Assumption A3 implies in turn that $\varepsilon_{k,k+m}$ tends to zero, and hence (3.10) holds. □

We note that Theorem 3.1 implies that B_k is necessarily positive definite for all k sufficiently large if $H(x_*)$ is positive definite.

Next we give the Q-superlinear rate of convergence properties of the MSR1.

Theorem 3.2. *Assume that Assumptions* A1–A4 *hold. Assume also that* $H(x_*)$ *is positive definite, and that* B_k *given in* (2.10) *is nonsingular and* $x_{k+1} = x_k + s_k$ *with* $s_k = -B_k^{-1}g_k$ *for all* k *sufficiently large. Then* $\{x_k\}$ *approaches* x_* *Q-superlinearly.*

Proof. We have

$$\frac{\|(B_k - H(x_*))s_k\|}{\|s_k\|} \leq \|B_k - H(x_*)\|.$$

Therefore, if Assumptions A1–A4 hold, then we obtain from Theorem 3.1 that

$$\lim_{k\to\infty} \frac{\|(B_k - H(x_*))s_k\|}{\|s_k\|} = 0.$$

This implies that the Dennis-Moré condition (see [4] for example) holds. Therefore the result holds. □

§4. MSR1 with trust region method

In the previous section, we considered the local behavior of the MSR1 under the assumption $x_k \to x_*$. However this assumption is not necessarily satisfied. In order to establish the global convergence of the method, we need to use globalization techniques like line search methods or trust region methods. The approximation matrix B_k generated by (2.10) is not always a positive definite matrix, and hence trust region methods are more appropriate to the MSR1 than line search methods.

In this section, we apply the trust region method proposed by Shultz et al. [13] to the MSR1. For this purpose, we give some definitions. For each iteration, to obtain step s_k, we approximately solve the following quadratic subproblem:

$$\min_{s\in R^n} m_k(s) = f(x_k) + g_k^T s + \frac{1}{2} s^T B_k s \qquad \text{subject to } \|s\| \leq \Delta_k,$$

where $\Delta_k > 0$ is the kth trust region radius. The approximate solution s_k is chosen such that

$$Pred_k \geq \sigma_1 \|g_k\| \min\{\Delta_k,\ \sigma_2\|g_k\|/\|B_k\|\} \tag{4.1}$$

holds for positive constants σ_1 and σ_2 and such that

$$\text{whenever } \|s_k\| < 0.8\Delta_k, \ \text{ then } B_k s_k = -g_k, \tag{4.2}$$

where $Pred_k$ is the predicted reduction, which is defined by

$$Pred_k = f(x_k) - m_k(s_k).$$

We also define the actual reduction by

$$Ared_k = f(x_k) - f(x_k + s_k).$$

Now we propose our algorithm, which follows the description of Algorithm 2.1 given by Byrd et al. [1].

Algorithm TRMSR1.

Step 0. Give $x_0 \in \boldsymbol{R}^n$*, an initial symmetric matrix* $B_0 \in \boldsymbol{R}^{n\times n}$*, an initial trust region radius* Δ_0*,* $\xi \in (0,\ 0.1)$*,* $\tau_1 \in (0,\ 1)$ *and* $\tau_2 > 1$*. Set* $k = 0$*.*

Step 1. Find a feasible approximate solution s_k *satisfying* (4.1) *and* (4.2) *to the subproblem*:

$$\min_{s\in R^n} \quad g_k^T s + \frac{1}{2} s^T B_k s \qquad \text{subject to } \|s\| \le \Delta_k.$$

Step 2. If $\dfrac{Ared_k}{Pred_k} > \xi$*, then set* $x_{k+1} = x_k + s_k$*, else set* $x_{k+1} = x_k$*.*

Step 3. If $\dfrac{Ared_k}{Pred_k} > 0.75$*,*

if $\|s_k\| < 0.8\Delta_k$*, then set* $\Delta_{k+1} = \Delta_k$*,*
else set $\Delta_{k+1} = \tau_2\Delta_k$*.*

Else

if $0.1 \le \dfrac{Ared_k}{Pred_k} \le 0.75$*, then set* $\Delta_{k+1} = \Delta_k$*,*

else set $\Delta_{k+1} = \tau_1\Delta_k$*.*

Step 4. Update B_k *by MSR1 update formula* (2.10)*.*

Step 5. Set $k = k + 1$ *and go to Step 1.*

Note that B_k is updated in Step 4, even if x_k is not updated (i.e. $x_{k+1} = x_k$). In [1, p.1028], the following comment is given: "Such updates along failed directions seem to be necessary to the convergence analysis because if the Hessian approximation is incorrect along such a direction and is not updated along that direction very similar directions could, in principle, be generated repeatedly at later iterations. Such steps would be rejected, resulting in the trust region being reduced at these iterations, potentially keeping it small enough that it would interfere with making a superlinear step even if the Hessian approximation is accurate enough to provide one."

Now we make the additional assumptions for the global convergence of Algorithm TRMSR1.

Assumption.

A5. The sequence $\{x_k\}$ *remains in a closed, bounded, convex set* D*. The objective function* f *has a unique stationary point* x_**, and* $H(x_*)$ *is positive definite.*

A6. The sequence of matrices $\{B_k\}$ *generated by the MSR1 update* (2.10) *is bounded, namely there exists a positive constant* c_4 *such that* $\|B_k\| \leq c_4$ *holds for all* k.

As stated before, note that Algorithm TRMSR1 is a trust region method of the type considered in Byrd et. al. [1], and the difference between their algorithm and Algorithm TRMSR1 is the update formula of B_k only. Moreover the global convergence theorem in Byrd et. al. [1, Theorem 2.1] follows from [13, Theorem 2.2] and its proof does not depend on update formulas of B_k. Accordingly, we give the following theorem without proof.

Theorem 4.1. *Suppose that Assumptions* A1, A2, A5 *and* A6 *hold. Let* $\{x_k\}$ *be the sequence generated by Algorithm* $TRMSR1$. *Then the sequence* $\{x_k\}$ *converges to* x_*.

In the rest of this section, we consider the rate of convergence of Algorithm TRMSR1. First, we give the following lemma that corresponds to [1, Lemma 2.3].

Lemma 4.1. *Let* $\{x_k\}$ *be a sequence of iterates which converges to the local solution* x_*, *and let* s_k *be a sequence of vectors such that* $x_k+s_k \to x_*$. *Assume that Assumptions* A1, A2, A5 *and* A6 *hold. Then there exists a nonnegative integer* K *such that for any set of* $n+1$ *steps,* $\mathcal{S} = \{s_{k_j} \mid K \leq k_1 < \cdots < k_{n+1}\}$, *there exist an index* k_m *with* $m \in \{2, 3, \ldots, n+1\}$ *and* M_3 *such that*

$$\frac{\|(B_{k_m} - H(x_*))s_{k_m}\|}{\|s_{k_m}\|} \leq M_3 \varepsilon_{k_1,k_{n+1}}^{1/n},$$

where

$$M_3 = 4\left[\sqrt{n}(L+\tau)\left\{\frac{1}{2} + \frac{1}{c_1}\left(1+\frac{2}{c_1}\right)^{k_{n+1}-k_1-2}\right\} + c_4 + \|H(x_*)\|\right].$$

Proof. The proof of this lemma is almost the same as the proof of [7, Lemma 3.2], and we only need to show that, for some positive M_4 that depends on $k_1, \ldots, k_{n+1}$,

$$\frac{\|(B_{k_j} - H(x_*))s_i\|}{\|s_i\|} \leq M_4 \varepsilon_{k_1,k_{n+1}} \tag{4.3}$$

holds for all $j = 2, \ldots, n+1$ and $i \in \{k_1, k_2, \ldots, k_{j-1}\}$. Similarly to (3.13), we have

$$\begin{aligned}
\frac{\|(B_{k_j} - H(x_*))s_i\|}{\|s_i\|} &\leq \frac{\|z_i - H(x_*)s_i\|}{\|s_i\|} + \frac{\|z_i - B_{k_j}s_i\|}{\|s_i\|} \\
&\leq (L+\tau)\varepsilon_{k_1,k_{n+1}} \\
&\quad + \frac{2}{c_1}(L+\tau)\left(1+\frac{2}{c_1}\right)^{k_{n+1}-k_1-2} \varepsilon_{k_1,k_{n+1}},
\end{aligned}$$

which implies (4.3) with $M_4 = (L+\tau)\{1 + \frac{2}{c_1}(1+2/c_1)^{k_{n+1}-k_1-2}\}$. □

Next we give a lemma which is obtained by applying Lemma 4.1 in a trust region context, and corresponds to [1, Lemma 2.4]. Its proof is the same as the proof of [1, Lemma 2.4], so we omit the proof.

Lemma 4.2. *Suppose that Assumptions* A1, A2, A5 *and* A6 *hold. Let* $\{x_k\}$ *be the sequence generated by Algorithm* TRMSR1*. Then there exists a nonnegative integer* N *such that, for any set of* p $(n < p)$ *steps* $s_{k+1}, s_{k+2}, \ldots, s_{k+p}$ *with* $k \geq N$*, there exists a set* $\mathcal{G}_k$ *of at least* $p-n$ *indices contained in the set* $\{i \mid k+1 \leq i \leq k+p\}$ *such that*

$$\frac{\|(B_j - H(x_*))s_j\|}{\|s_j\|} \leq M_5 \varepsilon_{k+1,k+p}^{1/n},$$

holds for all $j \in \mathcal{G}_k$*, where*

$$M_5 = 4\left[\sqrt{n}(L+\tau)\left\{\frac{1}{2} + \frac{1}{c_1}\left(1+\frac{2}{c_1}\right)^{p-2}\right\} + c_4 + \|H(x_*)\|\right].$$

Furthermore, for k *sufficiently large, if* $j \in \mathcal{G}_k$*, then*

$$\frac{Ared_j}{Pred_j} \geq 0.75.$$

This lemma implies that, in any set of p steps by Algorithm TRMSR1, there are at least $p-n$ steps accepted by Algorithm TRMSR1, and for which the approximate Hessian is accurate. Now we consider the local behaviors of Algorithm TRMSR1.

Theorem 4.2. *Suppose that Assumptions* A1, A2, A5 *and* A6 *hold. Let* $\{x_k\}$ *be the sequence generated by Algorithm TRMSR1. Then* $\{x_k\}$ *converges to* x_* $n+1$ *step Q-superlinearly, i.e.,* $\lim_{k\to\infty} \|x_{k+n+1} - x_*\|/\|x_k - x_*\| = 0$ *hold. Moreover, if Assumption* A4 *holds and* B_k *is nonsingular for all* k *sufficiently large, then* $\{x_k\}$ *converges to* x_* *Q-superlinearly.*

Proof. The $n+1$ step Q-superlinear convergence property of Algorithm TRMSR1 can be proven in the same way as Theorem 2.7 in [1]. This theorem is proven by using Lemmas 2.2–2.6 and Theorem 2.1 in [1], and these results do not depend on update formulas of B_k except Lemmas 2.3 and 2.4. We can use our Lemmas 4.1 and 4.2 instead of Lemmas 2.3 and 2.4 in [1] respectively to prove the $n+1$ step Q-superlinear convergence property of our method. Hence we omit the proof and we only prove the second result.

From Theorems 3.1 and 4.1, $\lim_{k\to\infty} \|B_k - H(x_*)\| = 0$ holds, and hence $\lim_{k\to\infty} \|B_k - \widehat{H}_k\| = 0$ also holds. Therefore, we have from $\xi \in (0,\ 0.1)$ that

$$\frac{Ared_k}{Pred_k} = \frac{g_k^T s_k + \frac{1}{2} s_k^T \widehat{H}_k s_k}{g_k^T s_k + \frac{1}{2} s_k^T B_k s_k} > \xi \tag{4.4}$$

holds for all k sufficiently large. Thus $\{x_k\}$ is updated by $x_{k+1} = x_k + s_k$ in Step 2 for all k sufficiently large. By (4.4) and Lemma 2.2 in [1], there exists a positive constant Δ such that

$$\Delta_k = \Delta \quad \text{and} \quad \|s_k\| < 0.8\Delta$$

for all k sufficiently large, and hence $\{x_k\}$ is updated by $x_{k+1} = x_k - B_k^{-1} g_k$. Therefore, from Theorem 3.2, the proof of the second result is complete. □

§5. Numerical results

In this section, we give some numerical results of Algorithm TRMSR1. We examined the following methods:

BFGS	: Algorithm TRMSR1 with BFGS update instead of MSR1,
SR1	: Algorithm TRMSR1 with SR1 update (namely $z_k = y_k$),
MSR1-1	: Algorithm TRMSR1 with (2.1) and $u_k = y_{k-1}$,
MSR1-2	: Algorithm TRMSR1 with (2.3) and $u_k = y_{k-1}$,
MSR1-3	: Algorithm TRMSR1 with (2.6) and $\nu_k = 0.01\|g_k\|$.

The test problems we used are described in Grippo et al. [6] and Moré et al. [12]. In Table 1, the first column, the second column and the third column denote the problem number in this paper, the problem name and the dimension of the problem, respectively. For each problem, we used the standard initial point x_0 given by [6] and [12].

The program was coded in JAVA 1.6, and computations were carried out on a Dell Precision 490 (Intel Xeon CPU 2.33GHz) with 4.0GB RAM. For these numerical experiments, we set $\Delta_0 = 1$, $\xi = 0.01$, $\tau_1 = 0.5$ and $\tau_2 = 2$ in Algorithm TRMSR1. We used the identity matrix I as an initial matrix B_0, and did an initial sizing. Specifically, in Step 4 of $k = 0$, we used $\tilde{B}_0 = (s_0^T z_0 / s_0^T s_0) I$ instead of $B_0 = I$ before updating B_0. For MSR1-1 and MSR1-2, if $|s_k^T u_k| \ge 10^{-15} \|s_k\| \|u_k\|$ was not satisfied, we set $z_k = y_k$. Moreover, if (3.1) with $c_1 = 10^{-8}$ did not hold, then we did not update B_k in Step 4 of Algorithm TRMSR1.

For solving a subproblem in Step 1, we used Hebden's method (see Algorithm 7.2.1 in [3], for example). In Hebden's method, if $\|B_k^{-1} g_k\| \ge 0.8\Delta_k$,

Table 1: Test problems

P	Name	Dimension n
1	Extended Rosenbrock function [12]	100
2	Extended Powell singular function [12]	100
3	Trigonometric function [12]	100
4	Oren function [6]	20
5	Dixon function [6]	10
6	Variably dimensioned function [12]	10
7	Wood function [12]	4
8	Helical valley function [12]	3
9	Cube function [6]	2
10	Freudenstein and Roth function [12]	2

nonlinear equation in μ

$$\frac{1}{\|(B_k + \mu I)^{-1} g_k\|} - \frac{1}{\Delta_k} = 0$$

is solved by the Newton method. We stopped the Newton method if (4.1) with $\sigma_1 = 0.1$ and $\sigma_2 = 0.75$ was satisfied.

The stopping condition was

$$\|g_k\| \leq 10^{-5}.$$

We also stopped the algorithm if the number of iterations exceeds 1000.

The numerical results of our experiment are reported in Table 2. The numerical results are given in the form of "the number of iterations / the number of inner iterations". Note that the number of inner iterations means sum of iterations of the Newton method in Step 1. If the number of iterations exceeds 1000, then we denote "*Failed* ".

We see from Table 2 that SR1 and MSR1-3 performed better than the other three methods in these limited numerical experiments: for Problem 1, SR1 outperformed MSR1-3; for Problem 3, MSR1-3 was superior to SR1; and for the other eight problems, MSR1-3 was comparable to SR1.

§6. Concluding remarks

In this paper, we treated SR1 method based on some modified secant conditions (MSR1) and investigated local behaviors of MSR1. In addition, we applied trust region methods to MSR1 to establish its global convergence. Although we used trust region methods in this paper, we can also consider MSR1

Table 2: Numerical results of Algorithm TRMSR1

P	n	BFGS	SR1	MSR1-1	MSR1-2	MSR1-3
1	100	87/54	78/56	42/59	65/23	213/167
2	100	91/5	53/13	73/52	69/29	54/25
3	100	46/0	180/117	85/5	97/32	71/7
4	20	544/2	187/2	183/4	188/2	190/2
5	10	217/116	67/16	*Failed*	*Failed*	60/14
6	10	23/2	23/2	23/2	24/2	25/2
7	4	89/3	44/43	135/43	35/3	43/44
8	3	12/6	18/24	85/28	95/118	19/27
9	2	73/17	48/33	*Failed*	68/44	45/30
10	2	42/6	16/4	19/5	17/5	17/4

with line search methods. Since the positive definiteness of the approximation matrix B_k is very important for line search methods, we need to establish $\widehat{r}_k^T s_k > 0$ for all k. By choosing q_k appropriately, we may be able to establish $\widehat{r}_k^T s_k > 0$ for all k. It is our further study.

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