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Convergence of a Positive Definite Symmetric Rank One Method with Restart

Abstract. We give the convergence result of a positive definite symmetric rank one with the line search method, namely +SSR1 method for unconstrained optimization. In general, the +SSR1 incorporates a restart procedure in the symmetric rank one (SR1) method. The restart procedure provides a replacement for the non-positive definite or unbounded (update with zero denominator) with a positive multiple of the identity matrix. However with this choice, the sequences of steps produced by the +SSR1 method may not usually seem to have the uniform linear independence property that is assumed in some convergence analysis for SR1. Therefore, we present an analysis that shows that the +SSR1 method with a line search is $n+1$ step $q-$superlinearly convergent without the assumption of linearly independent iterates. Our analysis only assumes that the Hessian approximations are positive definite and bounded asymptotically, which are the main features of the +SSR1 method. Computational experience shows that the +SSR1 method satisfies these requirements reasonably well in practice.

Key words. symmetric rank one, line search, restart, $q-$superlinearly convergent.
Mathematics Subject Classification. 65K10; 90C53

1. Introduction

We consider the quasi-Newton methods for finding a local minimum of the unconstrained optimization problem

$$\min f(x); \quad x \in \Re^n \tag{1}$$

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with $f(x)$ assumed to be at least twice continuously differentiable.

The algorithms for solving (1) are iterative with the basic framework of an iteration of a secant method described as follows:

Given the current iteration x_k, the gradient of the function at x_k, $\nabla f(x_k)$, and a symmetric $B_k \in \Re^{n\times n}$ (secant approximation to $\nabla^2 f(x_k)$), select the new iterate x_{k+1} by a line search method. Update B_{k+1} from B_k such that is B_{k+1} is symmetric and satisfies the secant equation $B_{k+1}s_k = y_k$, where $s_k = x_{k+1} - x_k$ and $y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$. In this paper, we consider the SR1 update for the Hessian approximation,

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{s_k^T(y_k - B_k s_k)}. \tag{2}$$

Throughout if $H = B^{-1}$, the inverse update respected to SR1 is given by

$$H_{k+1} = H_k + \frac{(s_k - H_k y_k)(s_k - H_k y_k)^T}{y_k^T(s_k - H_k y_k)}. \tag{3}$$

Minimization algorithms using this update in both a line search and trust region context have been shown in computational experiments by Conn et al. [2] and by Khalfan et al. [4] to be competitive with methods using the widely accepted BFGS update. However, the convergence of such algorithms is not as well understood, as convergence of the BFGS method. For instance, the BFGS method has been shown by Broyden et al. [1] to be locally q-superlinearly convergent provided that the initial Hessian approximation is sufficiently accurate. Powell [8] proved a global convergence result for the BFGS method when applied to strictly convex functions and used in conjunction with line searches that satisfy the Wolfe conditions (equations 6-7). A significant difference between the BFGS and SR1 updates that contributes to this situation is that while the BFGS algorithm is guaranteed to produce a positive definite B_{k+1} if B_k is positive definite and $s_k^T y_k > 0$, the SR1 update does not have this property. Furthermore, in practical implementations of a line search SR1 method, the Hessian approximations B_{k+1} may be indefinite at some iterations. Despite these drawbacks, Conn et al. [2] proved that the sequence of matrices generated by the SR1 updates converges to the actual Hessian $\nabla^2 f(x^*)$ at the minimizer x^*, provided that the sequence of steps taken, $\{s_k\}$ is uniformly linearly independent, which is where the denominator of the SR1 update is always sufficiently different from zero, and that the iterates converge to x^*. Using this result it is not difficult to prove that the rate of convergence is $q-$superlinear. The condition of linear independence of the sequence $\{s_k\}$ under which Conn et al. [2] analyze the performance of the SR1 method may be too strong in practice. On the other hand, a study by Khalfan et al. [4] for the SR1 in a line search context did not make a uniform linear independence assumption, and instead made the weaker assumptions that the matrices B_k are positive definite and uniformly bounded. Their analysis showed that the convergence rate of such iterates to be $n + 1-$step $q-$superlinear and $2n-$step

$q-$quadratic. Motivated by this analysis, Leong and Hassan [5] proposed a new SR1 line search methods, that is fairly standard with the suggested features (B_k are positive definite and uniformly bounded). Their approach is simple: a restart procedure is derived and used together with the SR1 method. The restart procedure provides a replacement for the non-positive definite or unbounded (indefinite) B_k with a positive multiple of the identity matrix. Many authors proposed modifications to the SR1 update to preserve the positive definiteness of B_k, see for examples [7], [9], [10]. The +SSR1 algorithm differs from other methods in which it did not attempt to modify the SR1 updating formula; instead it uses the standard SR1 updating formula with a restart. Hence, it is possible to extend the similar results of Khalfan et al. [4] to the +SSR1 method. In the next section, we present the algorithm of the +SSR1 method. Section 3 gives the convergence result of this method by requiring only the assumption of boundedness and positive definiteness of the Hessian approximation. Finally, computational examples are also given in Section 4.

2. Positive Definite Symmetric Rank One Method

We begin by describing the algorithm of the +SSR1 method:

+SSR1 Algorithm.

Step 0. Given an initial point x_0, an initial positive matrix $H_0 = I$, and set $k = 0$.

Step 1. If the convergence criterion

$$\|\nabla f(x_k)\| \leq \varepsilon \times \max\{1, \|x_k\|\} \tag{4}$$

is achieved, then stop.

Step 2. Compute a SR1 direction

$$p_k = -H_k \nabla f(x_k) \tag{5}$$

where H_k is assumed to be positive definite.

Step 3. Using a line search procedure, find an acceptable steplength, λ_k such that the Wolfe's conditions

$$f(x_k + \lambda_k p_k) \leq f(x_k) + \alpha_1 \lambda_k p_k^T \nabla f(x_k) \tag{6}$$

and

$$\nabla f(x_k + \lambda_k p_k)^T p_k \geq \alpha_2 p_k^T \nabla f(x_k) \tag{7}$$

are satisfied. ($\lambda_k = 1$ is always tried first, $0 < \alpha_1 < 0.5$ and $\alpha_1 < \alpha_2 < 1$)

Step 4. Set $x_{k+1} = x_k + \lambda_k p_k$.

Step 5. If $y_k^T s_k - y_k^T H_k y_k \leq 0$ (i.e. H_{k+1} might not be positive definite) or

$$| \, y_k^T (s_k - H_k y_k) \, | < r \|y_k\| \|s_k - H_k y_k\|, \tag{8}$$

where $r \in (0, 1)$,

or

$$\|H_k\|_\infty = \max_i \sum_j^n \mid a_{ij} \mid > L, \tag{9}$$

where a_{ij} is the element of H_k and L is a preset constant, then set $H_{k+1} = \delta_k I$, where

$$\delta_k = \frac{s_k^T s_k}{y_k^T s_k} - \left[\left(\frac{s_k^T s_k}{y_k^T s_k} \right)^2 - \frac{s_k^T s_k}{y_k^T y_k} \right]^{1/2}, \tag{10}$$

and subsequently let $p_{k+1} = -\delta_k \nabla f(x_{k+1})$. Else compute the next inverse Hessian approximation H_{k+1} by (3).

Step 7. Set $k := k+1$, and go to Step 1.

In Step 3, note that if $y_k^T s_k - s_k^T B_k s_k > 0$ is satisfied, then H_k is positive definite. However, if the condition is violated, H_k might still be positive definite provided that $y_k^T s_k - s_k^T B_k s_k > 0$. The latter condition requires B_k to be computed iteratively. Hence, it is not appropriate in our case. So, we opt for a more conservative approach to restart the update whenever $y_k^T s_k - s_k^T B_k s_k > 0$ to avoid indefinite cases. Furthermore, if H_k is not positive definite, it will be replaced by $\delta_{k-1} I$. The scaling δ_k, defined by (10) is derived by Leong and Hassan [5] in such a way that if H_{k+1} is updated from $H_k = \delta_{k-1} I$ using the SR1 formula, then H_{k+1} must be positive definite. In the next section we will show that for non-quadratic strictly convex functions, if the sequence $\{B_k\}$ (or $\{H_k\}$) remains positive definite and bounded, then the +SSR1 algorithm will generate at least p $q-$superlinear steps out of every $n+p$ steps. This will enable us to prove that convergence is $2n-$step $q-$quadratic. The basic idea behind this is that, if any step falls close enough to a subspace spanned by recent $m \leq n$ steps, then the Hessian approximation must be quite accurate in this subspace. Thus, if in addition the step is the full secant step $-H_k \nabla f(x_k)$, it should be a superlinear step. But in a line search method, for the step to be the full secant step, H_k must be positive definite. This property is guaranteed in the +SSR1 algorithm. In the following section we give the detail convergence results.

3. Convergence Rate of the SR1 without Uniform Linear Independence

Throughout this section the following assumptions will frequently be made:

Assumption 1 *i. The sequence of iterates $\{x_k\}$ remains in a closed, bounded, convex set D, on which the function f is twice continuously differentiable and has an unique minimizer at a point x^* such that its Hessian $\nabla^2 f(x^*)$ is positive definite, and $\nabla^2 f(x)$ is Lipschitz continuous near x^*, that is, there exists a constant $\gamma > 0$ such that for all x, y in some neighborhood of x^*,*

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq \gamma \|x - y\|. \tag{11}$$

ii. The sequence $\{x_k\}$ converges to x^*.

Firstly since +SSR1 method always generate positive definite H_k, then for a strongly convex objective function, a line search implementation with Wolfe conditions will ensure that Assumption 1 ii. holds.

Next we state the following result, which is due to Conn et al. [2]:

Lemma 1 *Let $\{x_k\}$ be a sequence of iterates defined by $x_{k+1} = x_k + s_k$ where $s_k = -\lambda_k B_k^{-1} \nabla f(x_k)$. Suppose that Assumption 1 holds, that the sequence of matrices $\{B_k\}$ is generated from the SR1 updates, and that for each iteration*

$$| s_k^T (y_k - B_k s_k) | < r \|s_k\| \|y_k - B_k s_k\| \tag{12}$$

where $r \in (0,1)$ is a constant. Then, for each j, $\|y_j - B_{j+1} s_j\| = 0$, and

$$\|y_j - B_i s_j\| \leq \frac{\gamma}{r} \left(\frac{2}{r} + 1 \right)^{i-j-2} \eta_{i,j} \|s_j\| \tag{13}$$

for all $i \geq j+2$, where $\eta_{i,j} = \max\{\|x_q - x_t\| : j \leq t \leq q \leq i\}$, and γ is the Lipschitz constant from Assumption 1.

Actually, it is apparent from Lemma 1 by Conn et al. [2] that, if the update is skipped (or replaced in the context of the +SSR1 method) whenever (12) is violated, then (13) still holds for all j in which (12) is true.

In the lemma below, given by Khalfan et al. [4] showed that if the sequence of steps generated by an iterative process using the SR1 update satisfies (12), and the sequence of matrices is bounded, then out of any set of $n+1$ steps, at least one is good. As in the previous lemma, condition (12) actually needs only hold at this set of $n+1$ steps, as long as the update is not made when that condition fails.

Lemma 2 *Suppose the assumptions of Lemma 1 are satisfied for the sequences $\{x_k\}$ and $\{B_k\}$, and that in addition there exists M for which $\|B_k\| \leq M$ for all k. Then there exist $K \geq 0$ with $S = \{s_{k_i} : K \leq k_1 \leq \ldots k_{n+1}\}$ and an index k_m, $m \in \{2, 3, \ldots, n+1\}$ such that*

$$\frac{\|(B_{k_m} - \nabla^2 f(x^*)) s_{k_m}\|}{\|s_{k_m}\|} < \bar{c} \varepsilon_M^{1/n} \tag{14}$$

where

$$\varepsilon_M = \max_{1 \leq j \leq n+1} \{\|x_j - x^*\|\} \tag{15}$$

and

$$\bar{c} = 4 \left[\gamma + \sqrt{n} \frac{\gamma}{r} \left(\frac{2}{r} + 1 \right)^{k_{n+1}+k_1-2} + M + \|\nabla^2 f(x^*)\| \right]. \tag{16}$$

We will also need the following lemma, which is similar to the well-known superlinear convergence characterization of Dennis and Moré [**?**].

Lemma 3 *Suppose the function f satisfies Assumption 1. If the quantities $e_k = \|x_k - x^*\|$ and $\frac{\|(B_k - \nabla^2 f(x^*))s_k\|}{\|s_k\|}$ are sufficiently small, and if $B_k s_k = -\nabla f(x_k)$, then*

$$\|x_k + s_k - x^*\| \leq \|\nabla^2 f(x^*)^{-1}\| \left[2\frac{\|(B_k - \nabla^2 f(x^*))s_k\|}{\|s_k\|} e_k + \frac{\gamma}{2} e_k^2 \right]. \quad (17)$$

Proof. See Khalfan et al. [4].

Using these lemmas one can show that for any $p > n$, +SSR1 algorithm will generate at least $p - n$ superlinear steps for every p iterations provided that B_k is positive definite. The following theorem is used to establish a rate of convergence for the +SSR1 algorithm under the assumptions that the sequence $\{B_k\}$ is bounded, satisfies (12) and stays positive definite.

Theorem 1. *Consider the sequence $\{x_k\}$ generated by the +SSR1 algorithm and suppose that Assumption 1 holds. If there exists K_0 such that B_k is positive definite for all $k \geq K_0$, then for any $p \geq n + 1$ there exists K_1 such that for all $k \geq K_1$,*

$$e_{k+p} \leq \alpha e_k^{p/n} \quad (18)$$

where α is a constant and $e_i = \|x_i - x^*\|$.

Proof. Since $\nabla^2 f(x^*)$ is positive definite, there exists K_1, $\beta_1 > 0$ and $\beta_2 > 0$ such that

$$\beta_1 \left(f(x_k) - f(x^*) \right)^{1/2} \leq \|x_k - x^*\| \leq \beta_2 \left(f(x_k) - f(x^*) \right)^{1/2} \quad (19)$$

for all $k \geq K_1$. Therefore since +SSR1 method is a descent method (This property is ensured by Step 3 of the +SSR1 algorithm and the Wolfe conditions), for all $l > k > K_1$ we have

$$\|x_l - x^*\| \leq \frac{\beta_2}{\beta_1} \|x_k - x^*\|. \quad (20)$$

Now we apply Lemma 2 to the set $\{s_k, s_{k+1}, \ldots, s_{k+n}\}$. Thus, there exist $l_1 \in \{k+1, \ldots, k+n\}$ such that

$$\frac{\|(B_{l_1} - \nabla^2 f(x^*))s_{l_1}\|}{\|s_{l_1}\|} < \bar{c} \left(\frac{\beta_2}{\beta_1} e_k \right)^{1/n}. \quad (21)$$

Equation (21) implies that for sufficiently small $\|x_{l_1} - x^*\|$ and by Lemma 3, we can choose a steplength λ_{l_1} in +SSR1 algorithm so that $x_{l_1+1} = x_{l_1} + s_{l_1}$. This fact, together with Lemma 3 and (21) implies that if e_k is sufficiently small then

$$e_{l_1+1} \leq \hat{\alpha} e_k^{1/n} e_{l_1} \quad (22)$$

for some constants $\hat{\alpha}$.

We may also apply Lemma 2 to the set $\{s_k, s_{k+1}, \ldots, s_{k+n}, s_{k+n+1}\} - \{s_{l_1}\}$ to get l_2. Hence, by repeating this step for $n-p$ times we get a set of integers $l_1 < l_2 < \ldots < l_{p-n}$ with $l_1 > k$ and $l_{p-n} < k+p$ such that

$$e_{l_i+1} \leq \hat{\alpha} e_k^{1/n} e_{l_i} \tag{23}$$

for each l_i. Suppose that $h_j = (f(x_j) - f(x^*))^{1/2}$. Since we have a descent method, it follows that

$$h_{j+1} \leq h_j. \tag{24}$$

Using 19 we have that for an arbitrary $k \geq K_1$,

$$\begin{aligned} h_{l_i+1} &\leq \frac{1}{\beta_1} e_{l_i+1} \\ &\leq \frac{\hat{\alpha}}{\beta_1} e_k^{1/n} e_{l_i} \\ &\leq \frac{\hat{\alpha}\beta_2}{\beta_1} e_k^{1/n} h_{l_i} \end{aligned} \tag{25}$$

for $i = 1, 2, \ldots, p-n$. Therefore using (19) and (24) we obtain

$$h_{k+p} \leq \left(\frac{\hat{\alpha}\beta_2}{\beta_1} e_k^{1/n} \right)^{p-n} h_k \tag{26}$$

which by (19) implies that

$$e_{k+p} \leq \frac{\beta_2}{\beta_1} \left(\frac{\hat{\alpha}\beta_2}{\beta_1} e_k^{1/n} \right)^{p-n} e_k. \tag{27}$$

Thus,

$$e_{k+p} \leq \hat{\alpha}^{p-n} \left(\frac{\beta_2}{\beta_1} \right)^{p-n+1} e_k^{p/n} \tag{28}$$

and the inequality (18) holds.

Finally, we give the rate of convergence for the +SSR1 algorithm:

Theorem 2. *Under the assumptions of Theorem 1, the sequence $\{x_k\}$ generated by the +SSR1 algorithm is $n+1-$step $q-$superlinear, i.e.,*

$$\liminf_{k\to\infty} \frac{e_{k+n+1}}{e_k} = 0, \tag{29}$$

and is $2n-$step $q-$quadratic, i.e.,

$$\limsup_{k\to\infty} \frac{e_{k+2n}}{e_k^2} \leq \infty. \tag{30}$$

Proof. Let $p = n+1$, and $p = 2n$, respectively in Theorem 1.

Note that one of the requirements in Theorem 1 for the rate of convergence to be $p-$step $q-$superlinear, is that the sequence $\{B_k\}$ generated by the SR1 method be positive definite and bounded. Generally, Theorem 1 only requires positive definiteness at the $p - n$ out of p "good iterations" (which is, steps where f is reduced). Eventually if $p = n + 1$ is chosen in Theorem 2, Theorem 1 actually requires positive definiteness at only 1 step out of $n + 1$ "good iterations". The +SSR1 algorithm satisfies this requirement because suppose that a non positive definite B_{k-1} is replaced by $\delta_k^{-1} I$ then B_{k+1} which is updated from $\delta_k^{-1} I$ must be positive definite. Hence, for every $n + 1$ steps greater that k, we will have at least 1 good step (which is, where B is positive definite and bounded). In the following section, we present computational results to illustrate the convergence of the +SSR1 method in practice.

4. Computational Results

We test the +SSR1 algorithm on a variety of test problems selected from Moré et al. [6]. The analytic gradients is used and the gradient stopping tolerance is 10^{-5}. All experiments are run using double precision arithmetic. For each test function, Table 1 reports the performance of the +SSR1 method. The table contains the followings: the test functions as given in [6], the dimension of the problem n, the number of iterations required to solve the problem n_I, the number of function and gradient evaluations required to solve the problem $n_{f/g}$ and the symbol "–" indicates that the number of iterations exceeds 999. We set 10^{-6} and $L = 10^8$ in Step 3 of the +SSR1 method, and $\alpha_1 = 10^{-4}$ and $\alpha_2 = 0.9$ within the Wolfe conditions (6)-(7). Numerical experiments on the performance of +SSR1 and BFGS method can be found in Leong and Hassan [7]. Hence in this paper, we give only the numerical results to illustrate the convergence of the +SSR1 method. The last two columns in Table 1 indicate the number of restarts that is due to non-positive definite of B_k (n_{res1}) and the number of restarts when either (8) or (9) is satisfied (n_{res2}). The results of Table 1 are summarized in Table 2.

From Table 2, we observe that the SR1 matrix is positive definite at least 70% of the time on every one of our test functions. In light of this, and since Theorem 1 really only requires positive definiteness at "good step", chances that superlinear steps will be taken at least every n steps by the algorithm seem good. In other words, we know that from Theorem 1 that out of every $2n$ steps, at least n will be "good steps" so long as B_k is positive definite at these iterations. The last column in Table 1, which reports the number of times (8) or (9) is satisfied, indicates that these conditions are rarely be satisfied in practice. This finding is consistent with the results of Khalfan et al. [4].

Table 1. Performance of the +SSR1 method

Test function (n)	n_I	$n_{f/g}$	n_{res1}	n_{res2}
Penalty I (4)	39	57	4	0
Penalty I (20)	47	80	4	0
Penalty I (100)	53	78	7	0
Penalty I (400)	60	82	3	0
Penalty II (4)	27	30	2	0
Penalty II (20)	212	325	28	0
Penalty II (100)	450	533	18	0
Penalty II (400)	–	–	–	–
Trigonometric (4)	14	21	1	0
Trigonometric (20)	61	88	9	0
Trigonometric (100)	56	84	15	0
Trigonometric (400)	75	117	21	0
Rosenbrook (4)	39	84	8	0
Rosenbrook (20)	82	132	18	0
Rosenbrook (100)	43	63	2	0
Rosenbrook (400)	62	89	11	0
Powell (4)	27	30	0	0
Powell (20)	27	31	0	0
Powell (100)	31	35	2	0
Powell (400)	33	40	3	0
Wood (4)	26	35	0	0
Wood (20)	35	52	3	0
Wood (100)	30	48	2	0
Wood (400)	61	84	13	0
Beale (4)	16	21	1	0
Beale (20)	18	27	2	0
Beale (100)	19	22	1	0
Beale (400)	14	18	0	0

Table 2. Percentage of iterations with H_k is positive definite

Percentage	<70	70-79	80-89	90-99	100
Number of test functions	0	5	6	12	4

5. Conclusions

We have attempted, in this paper, to investigate theoretical and numerical aspects of the +SSR1 formula for unconstrained optimization. We tested the +SSR1 method on a set of standard test problems from Moré et al. [6]. Our test results show that on the set of problems we tried, the +SSR1 method, is generally compliant to the results of Khalfan et al. [4]. Under conditions that do not assume uniform linear independence of the generated steps, but do assume positive definiteness and boundedness of the Hessian approximations, we were able to prove $n+1-$step $q-$superlinear convergence, and $2n-$step quadratic convergence, of a line search +SSR1 method.

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