Global Convergence of the Method of Shortest Residuals *

Yu-hong Dai and Ya-xiang Yuan

State Key Laboratory of Scientific and Engineering Computing,
Institute of Computational Mathematics and Scientific/Engineering Computing,
Chinese Academy of Sciences, P. O. Box 2719, Beijing 100080, P. R. China
Email address: dyh@indigo14.cc.ac.cn, yyx@lsec.cc.ac.cn.

Abstract

The method of shortest residuals (SR) was presented by Hestenes and studied by Pitlak. If the function is quadratic, and if the line search is exact, then the SR method reduces to the linear conjugate gradient method. In this paper, we put forward the formulation of the SR method when the line search is inexact. We prove that, if stepsizes satisfy the strong Wolfe conditions, both the Fletcher-Reeves and Polak-Ribière-Polyak versions of the SR method converge globally. When the Wolfe conditions are used, the two versions are also convergent provided that the stepsizes are uniformly bounded; if the stepsizes are not bounded, an example is constructed to show that they need not converge. Numerical results show that the SR method is a promising alternative of the standard conjugate gradient method.

Mathematics Subject Classification: 65k, 90c.

1. Introduction

The conjugate gradient method is particularly useful for minimizing functions of many variables

$$\min_{x\in\Re^n} \; f(x), \tag{1.1}$$

because it does not require to store any matrices. It is of the form

$$d_k = \begin{cases} -g_k, & \text{for } k=1; \\ -g_k + \beta_k d_{k-1}, & \text{for } k \geq 2, \end{cases} \tag{1.2}$$

$$x_{k+1} = x_k + \alpha_k d_k, \tag{1.3}$$

where $g_k = \nabla f(x)$, β_k is a scalar, and α_k is a stepsize obtained by a line search. Well-known formulas for β_k are called the Fletcher-Reeves (FR), Polak-Ribière-Polyak (PRP) formulas (see [1, 8, 9]. They are given by

$$\beta_k^{FR} = \frac{\|g_k\|^2}{\|g_{k-1}\|^2} \tag{1.4}$$

*This work was supported by National Science Foundation of China (19525101).

and

$$\beta_k^{PRP} = \frac{g_k^T(g_k - g_{k-1})}{\|g_{k-1}\|^2}, \tag{1.5}$$

where $\|\cdot\|$ is the Euclidean norm. This paper deals with another conjugate gradient method, the method of shortest residuals(SR).

The SR method was presented by Hestenes in his monograph [2] on conjugate direction methods. In the SR method the search direction d_k is taken as the shortest vector of the form

$$d_k = \frac{-g_k + \eta_k d_{k-1}}{1+\eta_k}, \qquad 0 < \eta_k < \infty, \tag{1.6}$$

where $d_1 = -g_1$. It follows that d_k is vertical to $g_k + d_{k-1}$, and hence its parameter satisfies the relation

$$(-g_k + \eta_k d_{k-1})^T(g_k + d_{k-1}) = 0. \tag{1.7}$$

Assuming that the line search is exact, Hestenes obtains the solution of (1.7):

$$\eta_k = \frac{\|g_k\|^2}{\|d_{k-1}\|^2}. \tag{1.8}$$

If the function is quadratic, and if the line search is exact, the vector d_{k+1} can be proved to be also the shortest residual in the k-simplex whose vertices are $-g_1, \cdots, -g_{k+1}$ (see [2]).

The SR method can be viewed as a special case of the conjugate subgradient method developed in Wolfe [14] and Lemaréchal [4] for minimizing a convex function which may be nondifferentiable. Based on this fact, Pitlak [7] also called the above as Wolfe-Lemaréchal method.

To investigate the equivalent form of the SR method for general functions and construct other conjugate gradient methods, Pitlak [7] introduces the family of methods:

$$d_k = -Nr\{g_k,\ -\beta_k d_{k-1}\}, \tag{1.9}$$

where $Nr\{a,\ b\}$ is defined as the point from a line segment spanned by the vectors a and b which has the smallest norm, namely,

$$\|Nr\{a,\ b\}\| = \min\{\|\lambda a + (1-\lambda)b\| : 0 \le \lambda \le 1\}. \tag{1.10}$$

If $g_k^T d_{k-1}$=0, one can solve (1.9) analytically and obtain

$$d_k = -(1-\lambda_k)g_k + \lambda_k \beta_k d_{k-1} \tag{1.11}$$

and

$$\lambda_k = \frac{\|g_k\|^2}{\|g_k\|^2 + \beta_k^2\|d_{k-1}\|^2}. \tag{1.12}$$

In this case, it is easy to see that direction d_k defined by (1.6) and (1.8) is corresponding to (1.11)-(1.12) with

$$\beta_k = 1. \tag{1.13}$$

Pitlak points out in [7] that if the line search is exact, and if $\beta_k \equiv 1$, the SR method is equivalent to the FR method, and the corresponding formula of β_k of the PRP method is

$$\beta_k = \frac{\|g_k\|^2}{|g_k^T(g_k - g_{k-1})|}. \tag{1.14}$$

One may argue that the corresponding formula of β_k of the PRP method should be

$$\beta_k = \frac{\|g_k\|^2}{g_k^T(g_k - g_{k-1})}. \tag{1.15}$$

Note that if the line search is exact, the reduced method by (1.15) will produce the same iterations as the PRP method. Powell [11]'s examples can also be used to show that the method may cycle without approaching any solution point even if the line search is exact. Thus we take (1.14) instead of (1.15).

For clarity, we now call method (1.3), (1.11) and (1.12) as the SR method provided that scalar β_k is such that the reduced method is the linear conjugate gradient method when the function is quadratic and the line search is exact. At the same time, we call formulae (1.13) and (1.14) for β_k as the FR and PRP versions of the SR method, and abbreviate them by FRSR and PRPSR respectively.

In this paper, we will investigate the convergence properties of the FRSR and PRPSR methods with the stepsize satisfying the Wolfe conditions:

$$f(x_k) - f(x_k + \alpha_k d_k) \geq -\delta \alpha_k g_k^T d_k, \tag{1.16}$$

$$g(x_k + \alpha_k d_k)^T d_k \geq \sigma g_k^T d_k, \tag{1.17}$$

or the strong Wolfe conditions, namely, (1.16) and

$$|g(x_k + \alpha_k d_k)^T d_k| \leq \sigma |g_k^T d_k|, \tag{1.18}$$

where $0 < \delta < \sigma < 1$. In [7], Pitlak suggests the following search conditions:

$$f(x_k) - f(x_k + \alpha_k d_k) \geq \delta \alpha_k \|d_k\|^2, \tag{1.19}$$

$$g(x_k + \alpha_k d_k)^T d_k \geq -\sigma \|d_k\|^2, \tag{1.20}$$

where $0 < \delta < \sigma < 1$, and he concludes that there exists a procedure which finds $\alpha_k > 0$ satisfying (1.19)-(1.20) in a finite number of operations (see Lemma 1 in [7]). However it is possible that $\hat{\alpha} = 0$ in his proof, the statement is not true. Consider

$$f(x) = \frac{1}{2}\epsilon x^2, \quad x \in \Re^1 \tag{1.21}$$

where $\epsilon > 0$ is constant. Suppose that at the k-th iteration $x_k = 1$ and $d_k = -1$ are obtained. Then for any $\alpha > 0$,

$$f(x_k) - f(x_k + \alpha d_k) = \frac{1}{2}\epsilon - \frac{1}{2}\epsilon(1-\alpha)^2 = \epsilon\alpha - \frac{1}{2}\epsilon\alpha^2. \tag{1.22}$$

The above implies that (1.19) does not hold for any $\alpha > 0$, provided that $\epsilon < \delta$. It is worth noting that, for the SR method, we often have that $g_k^T d_k = -\|d_k\|^2$, which implies that (1.19)-(1.20) are equivalent to (1.16)-(1.17).

This paper is organized as follows. In the next section, we give the formula of the SR method under inexact line searches and provide an algorithm in which some safeguards are employed. In Section 3, we prove that the FRSR and PRPSR algorithms converge with the strong Wolfe conditions (1.16) and (1.18). If the Wolfe conditions (1.16)-(1.17) are used, convergence is also guaranteed provided that the stepsizes are uniformly bounded. One direct corollary is that the FRSR and PRPSR algorithms with (1.16)-(1.17) converge for strictly convex functions. In Section 4, a function is constructed to show that, if we do not restrict $\{\alpha_k\}$, the Wolfe conditions can guarantee neither algorithms to converge. The example suits for both the FRSR and PRPSR algorithms. Numerical results are reported in Section 5, which show that the SR method is a promising alternative of the standard conjugate gradient method.

2. Algorithm

Expression (1.12) is deduced in the case of the exact line search. If the line search is inexact, it is not difficult to deduce from (1.9) that scalar λ_k in (1.11) is given by

$$\lambda_k = \frac{\|g_k\|^2 + \beta_k g_k^T d_{k-1}}{\|g_k + \beta_k d_{k-1}\|^2}, \tag{2.1}$$

if we do not restrict $\lambda_k \in [0,\ 1]$. By direct calculations, we can obtain

$$g_k^T d_k = -\|d_k\|^2 \tag{2.2}$$

and

$$\|d_k\|^2 = \frac{\beta_k^2 \left(\|g_k\|^2 \|d_{k-1}\|^2 - (g_k^T d_{k-1})^2\right)}{\|g_k + \beta_k d_{k-1}\|^2}. \tag{2.3}$$

It follows from (2.2) that d_k is a descent direction unless $d_k \neq 0$. On the other hand, from (2.3) we see that $d_k = 0$ if and only if g_k and d_{k-1} are collinear. In the case when g_k and d_{k-1} are collinear, assuming that $\beta_k d_{k-1} = t g_k$, we can solve d_k from (1.9) and (1.10) as follows:

$$d_k = \begin{cases} -g_k, & \text{if } t < -1; \\ t g_k, & \text{if } -1 \le t \le 0; \\ 0, & \text{if } t > 0. \end{cases} \tag{2.4}$$

The direction d_k vanishes if $t \geq 0$. The following example shows this possibility. Consider

$$f(x,y) = \frac{(1+\sigma)}{2}(x^2 + y^2). \tag{2.5}$$

Given the starting point $x_1 = (1,1)^T$, one can test the unit stepsize will satisfy (1.16) and (1.18) if the parameters δ and σ such that $\delta \le (1+\sigma)(1-\sigma^2)$. It follows that $x_2 = (-\sigma, -\sigma)^T$, and hence that $t = 1/\sigma$ for the FRSR method, $t = 1/(1+\sigma)$ for the PRPSR method. Thus we have $t > 0$ for both methods. In practice, to avoid numerical overflows we restart the algorithm with

$$d_k = -g_k \tag{2.6}$$

if the following condition is satisfied:

$$|g_k^T d_{k-1}| \ge b_1 \|g_k\| \|d_{k-1}\|, \tag{2.7}$$

where $b_1 \le 1$ is a positive number.

For the PRPSR method, it is obvious that the denominator of β_k possibly vanishes. Thus to establish convergence results for the PRPSR method we must assume that $|g_k^T (g_k - g_{k-1})| > 0$. In practice, we test the following condition at every iteration:

$$|g_k^T (g_k - g_{k-1})| > b_2 \|g_k\|^2, \tag{2.8}$$

where $0 \le b_2 < 1$.

Now we give a general algorithm as follows.

Algorithm 2.1 *Given a starting point* x_1. *Choose* $I \in \{0,\ 1\}$, *and numbers* $0 < b_1 \le 1$, $0 \le b_2 < 1$, $\epsilon \ge 0$.

Step 1. *Compute* $\|g_1\|$. *If* $\|g_1\| \le \epsilon$, *stop; otherwise, let* $k = 1$.

Step 2. *Compute* $d_k = -g_k$.

Step 3. *Find* $\alpha_k > 0$ *satisfying certain line search conditions.*

Step 4. *Compute* x_{k+1} *by (1.3) and* g_{k+1}. *Let* $k = k + 1$.

Step 5. *Compute* $\|g_k\|$. *If* $\|g_k\| \le \epsilon$, *stop.*

Step 6. *Test (2.7): if (2.7) does not hold, go to step (2). If* $I = 1$, *go to Step 8.*

Step 7. *Compute* β_k *by (1.13), go to Step 9.*

Step 8. *Test (2.8): if (2.8) does not hold, go to Step 2; compute* β_k *by (1.14).*

Step 9. *Compute* λ_k *by (2.1) and* d_k *by (1.11), go to Step 3.*

We call the above with $I = 0$ and $I = 1$ as the FRSR and PRPSR algorithms respectively.

3. Global Convergence

Throughout this section we make the following assumption.

Assumption 3.1 *(1)* f *is bounded below in* $\Re^n$ *and is continuously differentiable in a neighbor* $\mathcal{N}$ *of the level set* $\mathcal{L} = \{x \in \Re^n : f(x) \le f(x_1)\}$; *(2) The gradient* $\nabla f(x)$ *is Lipschitz continuous in* $\mathcal{N}$, *namely, there exists a constant* $L > 0$ *such that*

$$\|\nabla f(x) - \nabla f(y)\| \le L\|x - y\|, \text{ for any } x,\ y \in \mathcal{N}. \tag{3.1}$$

For some references, we formulate the following assumption.

Assumption 3.2 *The level set* $\mathcal{L} = \{x \in \Re^n : f(x) \le f(x_1)\}$ *is bounded.*

Note that Assumptions 3.1 and 3.2 imply that there is a constant $\overline{\gamma}$ such that

$$\|g(x)\| \le \overline{\gamma}, \qquad \text{for all } x \in \mathcal{L}. \tag{3.2}$$

We also formulate the following assumption.

Assumption 3.3 *The function* $f(x)$ *is twice continuously differentiable in* $\mathcal{N}$, *and there are numbers* $0 < \mu_1 \le \mu_2$ *such that*

$$\mu_1\|y\|^2 \le y^T H(x) y \le \mu_2\|y\|^2, \qquad \text{for all } x \in \mathcal{N} \text{ and } y \in \Re^n, \tag{3.3}$$

where $H(x)$ *denotes the Hessian matrix of* f *at* x.

Under Assumption 3.1, we state a useful result which was essentially proved by Zoutendijk [15] and Wolfe [12, 13].

Theorem 3.4 *Let x_1 be a starting point for which Assumption 3.1 is satisfied. Consider any iteration of the form (1.2), where d_k is a descent direction and α_k satisfies the Wolfe conditions (1.16)-(1.17). Then*

$$\sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty. \tag{3.4}$$

The above gives the following result:

Corollary 3.5 *Let x_1 be a starting point for which Assumption 3.1 is satisfied. Consider Algorithm 2.1 where $b_1 = 1,\ b_2 = 0$, $\epsilon = 0$, and where the line search conditions are (1.16)-(1.17). Then*

$$\sum_{k \geq 1} \|d_k\|^2 < \infty. \tag{3.5}$$

Proof If the algorithm restarts, we also have (2.2) due to (2.6). So Theorem 3.4 and relation (2.2) give the corollary. □

If Algorithm 2.1 restarts at the k-th iteration, we have $\|g_k\| = \|d_k\|$. Thus (3.5) implies $\liminf_{k\to\infty} \|g_k\| = 0$ if Algorithm 2.1 restarts for infinitely many times. Thus we suppose with loss of generality that (2.7) and (2.8) always hold in Algorithm 2.1. In addition, we also suppose that $g_k \neq 0$ for all k since otherwise a stationary point has been found. First, we have the following theorem for the FRSR method.

Theorem 3.6 *Let x_1 be a starting point for which Assumption 3.1 is satisfied. Consider Algorithm 2.1 with $I = 0$, $b_1 = 1$ and $\epsilon = 0$. Then we have that*

$$\liminf_{k\to\infty} \|g_k\| = 0, \tag{3.6}$$

if the line search satisfies one of the following conditions:

(i) $g_k^T d_{k-1} = 0$;

(ii) *the strong Wolfe conditions (1.16)-(1.18);*

(iii) *the Wolfe conditions (1.16)-(1.17), and there exists $M < \infty$ such that*

$$\alpha_k \leq M, \qquad \text{for all } k. \tag{3.7}$$

Proof We proceed by contradiction and assume that

$$\liminf_{k\to\infty} \|g_k\| \neq 0. \tag{3.8}$$

Then there exists a constant $\gamma > 0$ such that

$$\|g_k\| \geq \gamma, \qquad \text{for all } k \geq 1. \tag{3.9}$$

From (2.3) and (1.13), we obtain

$$\frac{1}{\|d_k\|^2} = \frac{1}{\|d_{k-1}\|^2}(1 + r_k), \tag{3.10}$$

where

$$r_k = \frac{\|d_{k-1}\|^2 + 2g_k^T d_{k-1} + \dfrac{(g_k^T d_{k-1})^2}{\|d_{k-1}\|^2}}{\|g_k\|^2 - \dfrac{(g_k^T d_{k-1})^2}{\|d_{k-1}\|^2}}. \tag{3.11}$$

Using (3.10) recursively, we get that

$$\frac{1}{\|d_k\|^2} = \frac{1}{\|d_1\|^2} \prod_{i=2}^{k} (1 + r_i). \tag{3.12}$$

Noting that $r_k > 0$, we deduce from (3.5) and (3.12) that

$$\sum_{k \geq 2} r_k = \infty \tag{3.13}$$

because otherwise we have that $1/\|d_k\|^2$ converges which contradicts with (3.5).

For (i), since $g_k^T d_{k-1} = 0$, r_k can be rewritten as

$$r_k = \frac{\|d_{k-1}\|^2}{\|g_k\|^2}. \tag{3.14}$$

From this and (3.9), we obtain

$$\sum_{k \geq 2} r_k \leq \frac{1}{\gamma} \sum_{k \geq 2} \|d_{k-1}\|^2 < \infty, \tag{3.15}$$

which contradicts (3.13);

For (ii) and (iii), we conclude that there exists a positive number c_1 such that for all $k \geq 2$,

$$|g_k^T d_{k-1}| \leq c_1 \|d_{k-1}\|^2. \tag{3.16}$$

In fact, for (ii), we see from (1.18) and (2.2) that (3.16) with $c_1 = \sigma$. For (iii), we have from (3.1), (2.2) and (3.7) that

$$\begin{aligned} |g_{k+1}^T d_k| &= |(g_{k+1} - g_k)^T d_k + g_k^T d_k| \\ &\leq \|g_{k+1} - g_k\| \|d_k\| + |g_k^T d_k| \\ &\leq \alpha_k L \|d_k\|^2 + \|d_k\|^2 \\ &\leq (1 + LM) \|d_k\|^2. \end{aligned} \tag{3.17}$$

So (3.16) holds with $c_1 = 1 + LM$. Due to (3.5), we see that

$$\|d_k\| \to 0, \qquad \text{as } k \to \infty, \tag{3.18}$$

which implies that there exists an integer k_1 such that

$$\|d_k\| \leq \frac{\sqrt{2}\gamma}{2c_1}, \qquad \text{for all } k \geq k_1. \tag{3.19}$$

Applying (3.16) and this in (3.11), we obtain for all $k \geq k_1$

$$r_k \leq c_2 \|d_{k-1}\|^2, \tag{3.20}$$

where $c_2 = 2(1 + c_1)^2/\gamma^2$. Therefore we also have that $\sum_{k \geq 2} r_k < \infty$, which contradicts (3.13). The contradiction shows the truth of (3.6). □

Corollary 3.7 *Let x_1 be a starting point for which Assumption 3.3 is satisfied. Consider Algorithm 2.1 with $I = 0$, $b_1 = 1$ and $\epsilon = 0$. Then if the line search satisfies (1.16)-(1.17), we have (3.6).*

Proof From (iii) of the above theorem, it suffices to show (3.7). By Taylor's theorem, we get that

$$f(x_k + \alpha d_k) = f(x_k) + \alpha g_k^T d_k + \frac{1}{2}\alpha^2 d_k^T H(\xi_k) d_k, \tag{3.21}$$

for some ξ_k. This, (1.16), (3.3) and (2.2) imply that (3.7) holds with $M = 2(1-\delta)/\mu_1$, which completes the proof. □

For the PRPSR method, we first have the following theorem.

Theorem 3.8 *Let x_1 be a starting point for which Assumption 3.1 are satisfied. Consider Algorithm 2.1 with $I = 1$, $b_1 = 1$, $b_2 = 0$ and $\epsilon = 0$. Then we have (3.6) if the line search satisfies (iii).*

Proof We still proceed by contradiction and assume that (3.9) holds. It is obvious that if the line search satisfies (iii), (3.16) still holds. From (1.14), (3.1), (3.7) and (3.9), we obtain

$$\beta_k \|d_{k-1}\| = \frac{\|g_k\|^2 \|d_{k-1}\|}{|g_k^T (g_k - g_{k-1})|} \geq \frac{\|g_k\|^2 \|d_{k-1}\|}{L\|g_k\| \alpha_{k-1} \|d_{k-1}\|} \geq c_3, \tag{3.22}$$

where $c_3 = \gamma/LM$. Using this and (3.9) in (2.3), we have the following estimation of $1/\|d_k\|^2$ for all $k \leq 1$:

$$\begin{aligned} \frac{1}{\|d_k\|^2} &= \left(\frac{1}{\beta_k^2 \|d_{k-1}\|^2} + \frac{2 g_k^T d_{k-1}}{\beta_k \|g_k\|^2 \|d_{k-1}\|^2} + \frac{1}{\|g_k\|^2}\right)\left(1 - \frac{(g_k^T d_{k-1})^2}{\|g_k\|^2 \|d_{k-1}\|^2}\right)^{-1} \\ &\leq 2\left(\frac{1}{\beta_k \|d_{k-1}\|} + \frac{1}{\|g_k\|}\right)^2 \left(1 - \frac{(g_k^T d_{k-1})^2}{\|g_k\|^2 \|d_{k-1}\|^2}\right)^{-1} \\ &\leq 2(c_3^{-1} + \gamma^{-1})^2 \left(1 - \frac{(g_k^T d_{k-1})^2}{\|g_k\|^2 \|d_{k-1}\|^2}\right)^{-1}. \end{aligned} \tag{3.23}$$

So

$$\sum_{k \geq 1} \left(1 - \frac{(g_k^T d_{k-1})^2}{\|g_k\|^2 \|d_{k-1}\|^2}\right) < \infty, \tag{3.24}$$

which implies

$$\liminf_{k \to \infty} \frac{(g_k^T d_{k-1})^2}{\|g_k\|^2 \|d_{k-1}\|^2} = 1. \tag{3.25}$$

Note that

$$g_{k-1} = g_k - y_{k-1}, \tag{3.26}$$

and

$$\liminf_{k \to \infty} \|y_{k-1}\| = \liminf_{k \to \infty} \alpha_{k-1} \|d_{k-1}\| = 0. \tag{3.27}$$

(3.25), (3.26) and (3.27) implies that

$$\liminf_{k\to\infty} \frac{(g_{k-1}^T d_{k-1})^2}{\|g_{k-1}\|^2\|d_{k-1}\|^2} = 1. \tag{3.28}$$

On the other hand, we have from (2.2), (3.9) and (3.18) that

$$\liminf_{k\to\infty} \frac{(g_{k-1}^T d_{k-1})^2}{\|g_{k-1}\|^2\|d_{k-1}\|^2} = \liminf_{k\to\infty} \frac{\|d_{k-1}\|^2}{\|g_{k-1}\|^2} = 0. \tag{3.29}$$

(3.28) and (3.29) give a contradiction. The contradiction shows the truth of (3.6). □

From Theorem 3.8, one can see that the PRPSR method also converges for strictly convex functions provided that stepsizes satisfy (1.16)-(1.17).

Corollary 3.9 *Let x_1 be a starting point for which Assumption 3.3 is satisfied. Consider Algorithm 2.1 with $I = 1$, $b_1 = 1$, $b_2 = 0$ and $\epsilon = 0$. Then if the line search satisfies (1.16)-(1.17), we have (3.6).*

Theorem 3.10 *Let x_1 be a starting point for which Assumptions 3.1 and 3.2 are satisfied. Consider Algorithm 2.1 with $I = 1$, $b_1 = 1$, $b_2 = 0$ and $\epsilon = 0$. Then we have (3.6) if the line search satisfies (1.16) and (1.18).*

Proof We proceed by contradiction and assume that (3.9) holds. At first, we conclude that there must exist a number c_4 such that

$$\beta_k\|d_{k-1}\| \le c_4, \qquad \text{for all } k \ge 1. \tag{3.30}$$

This is because otherwise there exists a subsequence $\{k_i\}$ and a constant, say also c_3, such that

$$\beta_{k_i}\|d_{k_i}\| \ge c_3, \qquad \text{for all } i \ge 1. \tag{3.31}$$

Then we can prove the truth of (3.23) for the subsequence $\{k_i\}$, which together with (3.5) implies that (3.25) still holds. Then similarly to the proof of Theorem 3.8, we can obtain (3.28) and (3.29), which contradicts with each other. Therefore (3.30) holds.

From (2.3), (3.19), (3.2) and (3.30), we can get that for all $k \ge k_1$

$$\|d_k\|^2 \ge \frac{\beta_k^2\|g_k\|^2\|d_{k-1}\|^2}{2\|g_k+\beta_k d_{k-1}\|^2} \ge \frac{\beta_k^2\|g_k\|^2\|d_{k-1}\|^2}{4(\|g_k\|^2+\beta_k^2\|d_{k-1}\|^2)} \ge c_5\beta_k^2\|d_{k-1}\|^2, \tag{3.32}$$

where $c_5 = \gamma^2/4(\overline{\gamma}^2 + c_4^2)$. Making products of both sides in (1.11) with d_k and applying (2.2), we can get

$$\beta_k d_{k-1}^T d_k = \|d_k\|^2. \tag{3.33}$$

Define $u_k = d_k/\|d_k\|$. Then from (3.33), $\beta_k \ge 0$, (2.3), (3.16) and (3.32), we obtain

$$\begin{aligned} \frac{1}{2}\|u_k - u_{k-1}\|^2 &= 1 - \frac{d_{k-1}^T d_k}{\|d_{k-1}\|\|d_k\|} = 1 - \frac{\|d_k\|}{\beta_k\|d_{k-1}\|} \\ &\le \frac{\beta_k^2\|d_{k-1}\|^2 - \|d_k\|^2}{\beta_k^2\|d_{k-1}\|^2} = \frac{(\beta_k\|d_{k-1}\|^2 + g_k^T d_{k-1})^2}{\|d_{k-1}\|^2\|g_k+\beta_k d_{k-1}\|^2} \\ &\le \frac{2\beta_k^2\|d_{k-1}\|^4 + 2(g_k^T d_{k-1})^2}{\|d_{k-1}\|^2\|g_k+\beta_k d_{k-1}\|^2} \le \frac{2c_5^{-1}\|d_k\|^2 + 2c_1^2\|d_{k-1}\|^2}{\|g_k+\beta_k d_{k-1}\|^2}. \end{aligned} \tag{3.34}$$

Besides it, from (1.18), (2.2) and (3.30),

$$\begin{aligned} \|g_k + \beta_k d_{k-1}\|^2 &\geq \|g_k\|^2 + 2\beta_k g_k^T d_{k-1} \\ &\geq \|g_k\|^2 - 2\beta_k \|d_{k-1}\|^2 \\ &\geq \|g_k\|^2 - 2c_4 \|d_{k-1}\|. \end{aligned} \tag{3.35}$$

Noting (3.5) and (3.9), we can deduce from (3.34) and (3.35) that

$$\sum_{k\geq 2} \|u_k - u_{k-1}\|^2 < \infty. \tag{3.36}$$

Let $|\mathcal{K}_{k,\Delta}^{\lambda}|$ denote the number of elements of

$$\mathcal{K}_{k,\Delta}^{\lambda} = \{i: \ k \leq i \leq k+\Delta-1, \|s_{i-1}\| = \|x_i - x_{i-1}\| > \lambda\}. \tag{3.37}$$

Using (3.36), we conclude that for any $\lambda > 0$, there exists $\Delta \in N^*$ and k_0 such that

$$|\mathcal{K}_{k,\Delta}^{\lambda}| \leq \frac{\Delta}{2}, \qquad \text{for any } k \geq k_0, \tag{3.38}$$

otherwise by the proof of Theorem 4.3 in [3] a contradiction can be similarly obtained. We choose $b = \gamma/2\overline{\gamma}$ and $\lambda = L\gamma/c_5^2 b$. Then we have from (3.2) and (3.9) that

$$\beta_k \geq \frac{\|g_k\|}{\|g_k\| + \|g_{k-1}\|} \geq \frac{\gamma}{2\overline{\gamma}} = b, \tag{3.39}$$

and when $\|s_{k-1}\| \leq \lambda$, we have from (3.1),

$$\beta_k \geq \frac{\|g_k\|}{L\|s_{k-1}\|} \geq \frac{\gamma}{L\lambda} = \frac{1}{c_5^2 b}, \tag{3.40}$$

For this λ, let Δ, k_0 be so given that (3.38) holds. Denote $q = [(k - k_1 + 1)/\Delta]$ and $t = k - k_1 + 1 - q\Delta$. It is obvious that $k - k_1 + 1 = q\Delta + t$ and $0 \leq t < \Delta$. Thus for any $k \geq k_2 = \max\{k_1, k_0\}$, we get from (3.32), and (3.38)-(3.40) that

$$\begin{aligned} \frac{\|d_k\|^2}{\|d_{k_1}\|^2} &\geq \prod_{i=k_1}^{k} (c_5\beta_i)^2 \geq \left[c_5^{q\Delta+t} b^{q\cdot\frac{\Delta}{2}+t} \left(\frac{1}{c_5^2 b}\right)^{q\cdot\frac{\Delta}{2}} \right]^2 \\ &= (c_5 b)^{2t} \geq \min\{c_5 b, \ (c_5 b)^{2\Delta}\}, \end{aligned} \tag{3.41}$$

which contradicts (3.18). The contradiction shows the truth of (3.6). □

4. A counter-example

In the above section, we prove that the FRSR and PRPSR algorithms converge with the Wolfe conditions (1.16)-(1.17) provided that $\{\alpha_k\}$ is uniformly bounded. However, if we do not restrict the size of α_k, they need not converge. This will be shown in the following example. The example suits for both algorithms.

Example 4. 1 Consider the function

$$f(x,y) = \begin{cases} 0, & \text{if } (x,y) = (0,0); \\ \frac{1}{4}\lambda(\frac{x}{\sqrt{x^2+y^2}})(x+y)^2 + \frac{1}{4}\lambda(\frac{y}{\sqrt{x^2+y^2}})(x-y)^2, & \text{otherwise}, \end{cases} \tag{4.1}$$

where λ is defined by

$$\lambda(t) = \begin{cases} 1, & \text{for } |t| > \frac{\sqrt{3}}{2}; \\ \frac{1}{2} + \frac{1}{2}\sin(b_1|t| + b_2), & \text{for } \frac{\sqrt{2}}{2} \le |t| \le \frac{\sqrt{3}}{2}; \\ 0, & \text{for } |t| < \frac{\sqrt{2}}{2}. \end{cases} \tag{4.2}$$

In (4.2), $b_1 = 2(\sqrt{3}+\sqrt{2})\pi$, $b_2 = -(5/2+\sqrt{6})\pi$. It is easy to see that function f defined by (4.1) and (4.2) satisfies Assumption 3.1.

We construct an example such that for all $k \ge 2$,

$$x_k = \|x_k\| \begin{pmatrix} \cos\frac{k-1}{2}\pi \\ \sin\frac{k-1}{2}\pi \end{pmatrix}, \tag{4.3}$$

$$\|x_k\| = \|x_{k-1}\| \tan(\frac{\pi}{4} - \tau_{k-1}), \quad \tau_{k-1} \in (0,\ \frac{\pi}{8}), \tag{4.4}$$

$$g_k = \frac{1}{2}\|x_k\| \begin{pmatrix} \cos(\frac{k-1}{2}\pi + \frac{\pi}{4}) \\ \sin(\frac{k-1}{2}\pi + \frac{\pi}{4}) \end{pmatrix}, \tag{4.5}$$

$$d_k = \|g_k\| \sin\tau_k \begin{pmatrix} \cos(\frac{k}{2}\pi + \frac{\pi}{4} + \tau_k) \\ \sin(\frac{k}{2}\pi + \frac{\pi}{4} + \tau_k) \end{pmatrix}. \tag{4.6}$$

Because we can use, for example spline fitting, we can choose the starting point and assume that (4.3)-(4.6) hold for $k = 2$. Suppose that (4.3)-(4.6) hold for k. From (4.3), (4.6) and the definition of f, we can choose $\alpha > 0$ such that

$$x_{k+1} = \|x_{k+1}\| \begin{pmatrix} \cos\frac{k}{2}\pi \\ \sin\frac{k}{2}\pi \end{pmatrix}, \tag{4.7}$$

$$\|x_{k+1}\| = \|x_k\| \tan(\frac{\pi}{4} - \tau_k). \tag{4.8}$$

Thus we have that

$$g_{k+1} = \frac{1}{2}\|x_{k+1}\| \begin{pmatrix} \cos(\frac{k}{2}\pi + \frac{\pi}{4}) \\ \sin(\frac{k}{2}\pi + \frac{\pi}{4}) \end{pmatrix}. \tag{4.9}$$

Since g_{k+1} is orthogonal to g_k, we have $g_{k+1}^T g_k = 0$ and hence $\beta_k = 1$ for both the FRSR and PRPSR algorithms. Defining $\eta_k = \lambda_k/(1-\lambda_k)$, where λ_k is given by (2.1), direct calculations show that

$$g_{k+1}^T d_k = \|g_{k+1}\|\|d_k\| \cos\tau_k, \tag{4.10}$$

$$\|g_{k+1}\| = \|g_k\| \tan(\frac{\pi}{4} - \tau_k), \tag{4.11}$$

$$\|d_k\| = \|g_k\| \sin\tau_k \tag{4.12}$$

and consequently

$$\begin{aligned} \eta_k &= \frac{\|g_{k+1}\|^2 + g_{k+1}^T d_k}{\|d_k\|^2 + g_{k+1}^T d_k} \\ &= \frac{\tan^2(\frac{\pi}{4} - \tau_k) + \cos\tau_k \tan(\frac{\pi}{4} - \tau_k)\sin\tau_k}{\cos\tau_k \tan(\frac{\pi}{4} - \tau_k)\sin\tau_k + \sin^2\tau_k} \\ &= \frac{\tan(\frac{\pi}{4} - \tau_k)}{\sin\tau_k}\xi_k, \end{aligned} \tag{4.13}$$

where

$$\xi_k = \cos\tau_k - \sin^3\tau_k + \cos\tau_k \sin^2\tau_k. \tag{4.14}$$

Therefore

$$\begin{aligned} d_{k+1} &= (1-\lambda_k)(-g_{k+1} + \eta_{k+1} d_k) \\ &= \gamma_k \left[\begin{pmatrix} \cos(\frac{k+2}{2}\pi + \frac{\pi}{4}) \\ \sin(\frac{k+2}{2}\pi + \frac{\pi}{4}) \end{pmatrix} + \xi_k \begin{pmatrix} \cos(\frac{k+2}{2}\pi + \frac{\pi}{4} + \tau_k) \\ \sin(\frac{k+2}{2}\pi + \frac{\pi}{4} + \tau_k) \end{pmatrix} \right], \end{aligned} \tag{4.15}$$

where $\gamma_k = (1-\lambda_k)\tan(\frac{\pi}{4} - \tau_k)\|g_k\|$. Noting that $\xi_k \geq 1$ for all $\tau_k \in (0,\ \pi/8)$, the above relation indicates that

$$\frac{d_{k+1}}{\|d_{k+1}\|} = \begin{pmatrix} \cos(\frac{k+1}{2}\pi + \frac{\pi}{4} + \tau_{k+1}) \\ \sin(\frac{k+1}{2}\pi + \frac{\pi}{4} + \tau_{k+1}) \end{pmatrix} \tag{4.16}$$

and

$$-\frac{\pi}{4} + \tau_k \leq \tau_{k+1} \leq \frac{\tau_k}{2}. \tag{4.17}$$

Because $d_{k+1}^T g_{k+1} < 0$, we have that

$$0 < \tau_{k+1} \leq \frac{\tau_k}{2}. \tag{4.18}$$

Again we have $\tau_{k+1} \in (0,\ \frac{\pi}{8})$. Because $d_{k+1}^T g_{k+1} = -\|d_{k+1}\|^2$, we have

$$d_{k+1} = \|d_{k+1}\| \sin\tau_{k+1} \begin{pmatrix} \cos(\frac{k+1}{2}\pi + \frac{\pi}{4} + \tau_{k+1}) \\ \sin(\frac{k+1}{2}\pi + \frac{\pi}{4} + \tau_{k+1}) \end{pmatrix}. \tag{4.19}$$

By induction, we have (4.3)-(4.6) hold for all $k \geq 2$. Now we test whether (1.16)-(1.17) hold. First, due to $g_{k+1}^T d_k > 0$, (1.17) obviously holds. Further, from (2.2), (4.3) and (4.5), we have

$$-\alpha_k g_k^T d_k = \alpha_k \|d_k\|^2 = \|d_k\|\|x_{k+1} - x_k\| = \frac{2\|g_k\|\|d_k\|}{\cos\tau_k + \sin\tau_k}. \tag{4.20}$$

By the definition of f, (4.11) and (4.12),

$$\begin{aligned} f_k - f_{k+1} &= \frac{1}{2}(\|g_k\|^2 - \|g_{k+1}\|^2) = \frac{1}{2}\|g_k\|^2 \left[1 - \tan^2(\frac{\pi}{4} - \tau_k)\right] \\ &= \frac{2\cos\tau_k \sin\tau_k}{(\cos\tau_k + \sin\tau_k)^2}\|g_k\|^2 = \frac{2\cos\tau_k \|g_k\|\|d_k\|}{(\cos\tau_k + \sin\tau_k)^2} \\ &\triangleq -\delta_k \alpha_k g_k^T d_k, \end{aligned} \tag{4.21}$$

where

$$\delta_k = \frac{\cos\tau_k}{\cos\tau_k + \sin\tau_k}. \tag{4.22}$$

Note that (4.18) implies that

$$\tau_k \to 0, \qquad \text{as } k \to \infty. \tag{4.23}$$

The above two relations indicate that for any positive number $\delta < 1$, $\delta_k > \delta$ for large k. Therefore, if we choose a suitable starting point, (1.16) and (1.17) hold for any $0 < \sigma < \delta < 1$.

However, from (4.4) and (4.18), one can prove that

$$\|x_k\| = \|x_2\| \prod_{i=2}^{k-1} \tan(\frac{\pi}{4} - \tau_i) \to c_6\|x_2\|, \quad \text{as } k \to \infty \tag{4.24}$$

where $c_6 = \prod_{i=1}^{\infty} \tan(\frac{\pi}{4} - \tau_i) > 0$. Thus any cluster point of $\{x_k\}$ is a non-stationary point.

In this example, we have from (4.20) that

$$\alpha_k = \frac{2\|g_k\|}{(\cos\tau_k + \sin\tau_k)\|d_k\|} = \frac{2}{(\cos\tau_k + \sin\tau_k)\sin\tau_k}, \tag{4.25}$$

which, together with (4.23), implies that

$$\alpha_k \to \infty, \qquad \text{as } k \to \infty. \tag{4.26}$$

The above example shows that if we only impose (1.16)-(1.17) on every line search, it is possible that $\{\alpha_k\}$ is not bounded, and the FRSR and PRPSR algorithms fail.

5. Numerical results

We tested the FRSR and PRPSR algorithms on SGI Indigo workstations. Our line search subroutine computes α_k such that (1.16) and (1.18) hold for $\delta = 0.01$ and $\sigma = 0.1$. The initial value of α_k is always set to 1. Although in this case the convergence results, i. e., Theorems 3.6 and 3.10 hold for any numbers $0 < b_1 \leq 1$ and $0 \leq b_2 < 1$, we choose $b_1 = 0.9$ and $b_2 = 0.1$ to avoid numerical overflows.

We compared the numerical results of our algorithms with the Fletcher-Reeves method and the Polak-Ribière-Polyak method. For the PRP algorithm, we restart it by setting $d_k = -g_k$ whenever a down-hill search direction is not produced.

We tested the algorithms on the 18 examples given by Morè, Garbow and Hillstrom [6]. The results are reported in Table 4.1. The column "P" denotes the number of the problems, and "N" the number of variables. The numerical results are given in the form of I/F/G, where I, F, G are numbers of iterations, function evaluations, and gradient evaluations respectively. The stopping condition is

$$\|g_k\| \leq 10^{-6}. \tag{5.1}$$

The algorithms are also terminated if the number of function evaluations exceed 5000. We also terminate the calculation if the function value improvement is too small. More exactly, algorithms are terminated whenever

$$[f(x_k) - f(x_{k+1})]/[1 + |f(x_k)|]) \leq 10^{-16}. \tag{5.2}$$

Table 4.1

P	N	FRSR	PRPSR	FR	PRP
1	3	90/266/116	53/168/78	106/358/133	61/224/93
2	6	302/768/743	158/395/375	317/816/434	126/265/205
3	3	3/7/5	3/7/5	3/7/5	3/7/5
4	2	>5000	*Failed*	>5000	*Failed*
5	3	27/71/63	9/31/26	>5000	13/39/29
6	6	3/16/7	3/16/7	3/16/7	3/15/9
7	9	662/2077/1899	>5000	1424/4311/1456	>5000
8	8	30/122/113	30/130/118	28/81/56	*Failed*
9	3	29/69/46	12/29/19	15/40/24	10/28/18
10	2	*Failed*	14/56/21	*Failed*	*Failed*
11	4	36/167/52*	*Failed*	*Failed*	31/152/52*
12	3	*Failed*	84/278/230	>5000	579/1687/965
13	20	>5000	61/125/125	>5000	53/106/102
14	14	63/213/116	44/153/91	151/583/240	22/104/59
15	16	1449/3102/2899	41/119/65	>5000	187/569/247
16	2	22/59/40	19/53/36	32/92/45	9/28/16
17	4	>5000	49/169/86	1136/4737/1306	140/589/265
18	8	781/2164/1029	47/125/71	613/2014/728	28/81/39

In the table, a superscript "*" indicates that the algorithm terminated due to (5.2) but (5.1) is not satisfied, and "*Failed*" means that d_k is so small that a numerical overflow happens while the algorithm tries to compute $f(x_k + d_k)$.

From Table 4.1, We found that the FRSR and PRPSR algorithms perform better than the Fletcher-Reeves and Polak-Ribière-Polyak algorithms respectively. Therefore, the SR method will be a promising alternative of the standard conjugate gradient method.

It is known that if a very small step is produced by the FR method, then this behavior may continue for a very large number of iterations unless the method is restarted. This behavior was observed and explained by Powell [10], Gilbert and Nocedal [3]. In fact, the statement is also true for the FRSR method. Let θ_k denote the angle between $-g_k$ and d_k. It follows from the definition of θ_k and (1.12) that

$$\cos\theta_k = \frac{-g_k^T d_k}{\|g_k\|\|d_k\|} = \frac{\|d_k\|}{\|g_k\|}. \tag{5.3}$$

Suppose that at k-iteration a "bad" search direction is generated, such that $\cos\theta_k \approx 0$, and that $x_{k+1} \approx x_k$. Thus $\|g_{k+1}\| \approx \|g_k\|$, and by (5.3),

$$\|d_k\| \ll \|g_k\| \approx \|g_{k+1}\|. \tag{5.4}$$

From (2.1), (1.13), (1.18) and this, we see that

$$\lambda_k \to 1, \text{ as } k \to \infty, \tag{5.5}$$

which with (1.11) implies that

$$d_{k+1} \approx d_k. \tag{5.6}$$

Hence, by this and (5.4),

$$\|d_{k+1}\| \ll \|g_{k+1}\|, \tag{5.7}$$

which together with (5.3) shows that $\cos\theta_{k+1} \approx 0$. The argument can therefore start all over again.

Acknowledgements. The authors were very grateful to the referees for their valuable comments and suggestions.

References

[1] Fletcher R. and Reeves C. (1964), *Function minimization by conjugate gradients*, Comput. J. **7**, 149-154.

[2] Hestenes M. R. (1980), *Conjugate direction methods in optimization*, Springer-Verlag, New York Heidelberg Berlin, 241-247.

[3] Gilbert J. C. and Nocedal J. (1992), *Global convergence properties of conjugate gradient methods for optimization*, SIAM. J. Optimization. **2** (1), 21-42.

[4] Lemaréchal C. (1975), *An extension of Davidon methods to nondifferentiable problems*, Mathematical Programming Study **3**, 95-109.

[5] McCormick G. P. and Ritter K. (1975), *Alternative Proofs of the convergence properties of the conjugate-gradient method*, JOTA: VOL. 13, NO. **5**, 497-518

[6] Morè J. J., Garbow B. S. and Hillstrom K. E. (1981), *Testing unconstrained optimization software*, ACM Transactions on Mathematical Software **7**, 17-41

[7] Pitlak R. (1989), *On the convergence of conjugate gradient algorithm*, IMA Journal of Numerical Analysis **14**, 443-460.

[8] Polak E. and Ribière G. (1969), *Note sur la convergence de directions conjugées*, Rev. Francaise Informat Recherche Operationelle, 3e Année **16**, 35-43.

[9] Polyak B. T. (1969), *The conjugate gradient method in extremem problems*, USSR Comp. Math. and Math. Phys. **9**, 94-112.

[10] Powell M. J. D. (1977), *Restart procedures of the conjugate gradient method*, Math. Program. **2**, 241-254.

[11] Powell M. J. D. (1984), *Nonconvex minimization calculations and the conjugate gradient method*, in: Lecture Notes in Mathematics vol. **1066**, Springer-Verlag (Berlin) (1984), pp. 122-141.

[12] Wolfe P. (1969), *Convergence conditions for ascent methods*, SIAM Review **11**, 226-235.

[13] Wolfe P. (1971), *Convergence conditions for ascent methods. II: Some corrections*, SIAM Review **13**, 185-188.

[14] Wolfe P. (1975), *A method of conjugate subgradients for minimizing nondifferentiable functions*, Math. Prog. Study **3**, 145-173.

[15] Zoutendijk G. (1970), *Nonlinear Programming, Computational Methods*, in: Integer and Nonlinear Programming (J.Abadie,ed.), North-Holland (Amsterdam), 37-86.