

A NONLINEAR CONJUGATE GRADIENT METHOD WITH A STRONG GLOBAL CONVERGENCE PROPERTY*

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Abstract. Conjugate gradient methods are widely used for unconstrained optimization, especially large scale problems. The strong Wolfe conditions are usually used in the analyses and implementations of conjugate gradient methods. This paper presents a new version of the conjugate gradient method, which converges globally, provided the line search satisfies the standard Wolfe conditions. The conditions on the objective function are also weak, being similar to those required by the Zoutendijk condition.

Key words. unconstrained optimization, new conjugate gradient method, Wolfe conditions, global convergence

AMS subject classifications. 65K, 90C

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1. Introduction. Our problem is to minimize a function of n variables

$$(1.1) \quad f(x),$$

where f is smooth and its gradient $g(x)$ is available. Conjugate gradient methods for solving (1.1) are iterative methods of the form

$$(1.2) \quad x_{k+1} = x_k + \alpha_k d_k,$$

where $\alpha_k > 0$ is a steplength and d_k is a search direction. Normally the search direction at the first iteration is the steepest descent direction, namely, $d_1 = -g_1$. The other search directions can be defined recursively:

$$(1.3) \quad d_{k+1} = -g_{k+1} + \beta_k d_k.$$

$\beta_k \in \mathfrak{R}$ is so chosen that (1.2)–(1.3) reduces to the linear conjugate gradient method if $f(x)$ is a strictly convex quadratic function and if α_k is the exact one-dimensional minimizer. Well-known formulas for β_k are the Fletcher–Reeves (FR), Polak–Ribière–Polyak (PRP), and Hestenes–Stiefel (HS) formulas (see [6]; [10], [11]; and [7], respectively) and are given by

$$(1.4) \quad \beta_k^{FR} = \|g_{k+1}\|^2 / \|g_k\|^2,$$

$$(1.5) \quad \beta_k^{PRP} = g_{k+1}^T y_k / \|g_k\|^2,$$

$$(1.6) \quad \beta_k^{HS} = g_{k+1}^T y_k / d_k^T y_k,$$

where $y_k = g_{k+1} - g_k$ and $\|\cdot\|$ denotes the Euclidean norm.

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The global convergence properties of the FR, PRP, and HS methods without regular restarts have been studied by many authors, including Zoutendijk [15], Al-Baali [1], Liu, Han, and Yin [9], Dai and Yuan [2], Powell [12], Gilbert and Nocedal [8], and Dai and Yuan [4]. To establish the convergence results of these methods, it is normally required that the steplength α_k satisfy the following strong Wolfe conditions:

$$(1.7) \quad f(x_k) - f(x_k + \alpha_k d_k) \geq -\delta \alpha_k g_k^T d_k,$$

$$(1.8) \quad |g(x_k + \alpha_k d_k)^T d_k| \leq -\sigma g_k^T d_k,$$

where $0 < \delta < \sigma < 1$. Some convergence analyses even require the α_k be computed by the exact line search, namely,

$$(1.9) \quad f(x_k + \alpha_k d_k) = \min_{\alpha > 0} f(x_k + \alpha d_k).$$

On the other hand, many other numerical methods for unconstrained optimization are proved to be convergent under the standard Wolfe conditions (1.7) and

$$(1.10) \quad g(x_k + \alpha_k d_k)^T d_k > \sigma g_k^T d_k.$$

For example, see Fletcher [5]. Hence it is interesting to investigate whether there exists a conjugate gradient method that converges under the standard Wolfe conditions.

In this paper, we give a new formula for β_k . It is shown that this new conjugate gradient method is globally convergent as long as the standard Wolfe conditions (1.7) and (1.10) are satisfied. Moreover, the conditions on the objective function are also weaker than the usual ones.

2. New formula for β_k . One motivation for our new formula for β_k is the descent property of the conjugate descent method (see Fletcher [5]), which uses

$$(2.1) \quad \beta_k^{CD} = \|g_{k+1}\|^2 / (-d_k^T g_k).$$

It can be shown that the conjugate descent method always produces a descent direction if the strong Wolfe conditions are satisfied. We try to find a conjugate gradient method which generates descent directions provided the standard Wolfe conditions are satisfied. Suppose the current search direction d_k is a descent direction, namely, $d_k^T g_k < 0$. Now we need to find a β_k that defines a descent direction d_{k+1} . This requires that

$$(2.2) \quad -\|g_{k+1}\|^2 + \beta_k g_{k+1}^T d_k < 0.$$

We assume that $\beta_k > 0$. Denote $\tau_k = \|g_{k+1}\|^2 / \beta_k$. The above inequality is equivalent to

$$(2.3) \quad \tau_k > g_{k+1}^T d_k.$$

Therefore, we can let $\tau_k = d_k^T y_k$, giving our new formula

$$(2.4) \quad \beta_k = \|g_{k+1}\|^2 / d_k^T y_k.$$

This formula is well defined because line search condition (1.10) implies $d_k^T y_k > 0$. If line searches are exact, the above formula is the same as the FR formula (1.4). Therefore we see that (2.4) corresponds to a nonlinear conjugate gradient method. It is interesting to note that (2.4) has the same numerator as the FR formula (1.4) and has the same denominator as the HS formula (1.6). Now we can define the new method, as follows.

ALGORITHM 2.1 (A new CG method).

Step 1. Given $x_1 \in \mathfrak{R}^n$, $d_1 = -g_1$, $k := 1$, if $g_1 = 0$, then stop.

Step 2. Compute an $\alpha_k > 0$ satisfying (1.7) and (1.10).

Step 3. Let $x_{k+1} = x_k + \alpha_k d_k$. If $g_{k+1} = 0$, then stop.

Step 4. Compute β_k by (2.4) and generate d_{k+1} by (1.3),
 $k := k + 1$, go to Step 2.

It follows from (1.3) and (2.4) that

$$(2.5) \quad g_{k+1}^T d_{k+1} = \frac{\|g_{k+1}\|^2}{d_k^T y_k} g_k^T d_k = \beta_k g_k^T d_k.$$

The above relation can be rewritten as

$$(2.6) \quad \beta_k = \frac{g_{k+1}^T d_{k+1}}{g_k^T d_k}.$$

This formula is very important in our convergence analysis.

3. Convergence of the new method. In this section, we establish a convergence theorem for Algorithm 2.1. We assume that the objective function satisfies the following conditions.

Assumption 3.1. (1) f is bounded below on \mathfrak{R}^n and is continuously differentiable in a neighborhood \mathcal{N} of the level set $\mathcal{L} = \{x \in \mathfrak{R}^n : f(x) \leq f(x_1)\}$; (2) the gradient $\nabla f(x)$ is Lipschitz continuous in \mathcal{N} , i.e., there exists a constant $L > 0$ such that

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

Under Assumption 3.1, we give a useful lemma which was essentially proved by Zoutendijk [15] and Wolfe [13, 14].

LEMMA 3.2. *Suppose that x_1 is a starting point for which Assumption 3.1 is satisfied. Consider any method of the form (1.2), where d_k is a descent direction and α_k satisfies the standard Wolfe conditions (1.7) and (1.10). Then we have that*

$$(3.2) \quad \sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty.$$

Proof. It follows from (1.10) that

$$(3.3) \quad d_k^T y_k = d_k^T (g_{k+1} - g_k) \geq (\sigma - 1)g_k^T d_k.$$

On the other hand, the Lipschitz condition (3.1) implies

$$(3.4) \quad (g_{k+1} - g_k)^T d_k \leq \alpha_k L \|d_k\|^2.$$

The above two inequalities give

$$(3.5) \quad \alpha_k \geq \frac{\sigma - 1}{L} \cdot \frac{g_k^T d_k}{\|d_k\|^2},$$

which with (1.7) implies that

$$(3.6) \quad f_k - f_{k+1} \geq c \frac{(g_k^T d_k)^2}{\|d_k\|^2},$$

where $c = \delta(1 - \sigma)/L$. Summing (3.6) and noting that f is bounded below, we see that (3.2) holds, which concludes the proof. \square

THEOREM 3.3. *Suppose that x_1 is a starting point for which Assumption 3.1 holds. Let $\{x_k, k = 1, 2, \dots\}$ be generated by Algorithm 2.1. Then the algorithm either terminates at a stationary point or converges in the sense that*

$$(3.7) \quad \liminf_{k \rightarrow \infty} \|g_k\| = 0.$$

Proof. If the algorithm does not terminate after finite many iterations, we have that

$$(3.8) \quad \|g_k\| > 0 \quad \text{for all } k.$$

First we show all search directions are descent, namely,

$$(3.9) \quad g_k^T d_k < 0$$

for all k . The above inequality is obvious for $k = 1$. Now we prove it for all $k \geq 1$ by induction. Assume (3.9) holds for k . It follows from the line search conditions that

$$(3.10) \quad d_k^T y_k \geq (\sigma - 1)d_k^T g_k > 0.$$

The above inequality and (2.5) imply that (3.9) holds for $k + 1$. This shows that (3.9) is true for all $k \geq 1$.

We now rewrite (1.3) as

$$(3.11) \quad d_{k+1} + g_{k+1} = \beta_k d_k.$$

Squaring both sides of the above equation, we get

$$(3.12) \quad \|d_{k+1}\|^2 = \beta_k^2 \|d_k\|^2 - 2g_{k+1}^T d_{k+1} - \|g_{k+1}\|^2.$$

Dividing both sides by $(g_{k+1}^T d_{k+1})^2$ and applying (2.6), we obtain that

$$(3.13) \quad \begin{aligned} \frac{\|d_{k+1}\|^2}{(g_{k+1}^T d_{k+1})^2} &= \frac{\|d_k\|^2}{(g_k^T d_k)^2} - \frac{2}{g_{k+1}^T d_{k+1}} - \frac{\|g_{k+1}\|^2}{(g_{k+1}^T d_{k+1})^2} \\ &= \frac{\|d_k\|^2}{(g_k^T d_k)^2} - \left(\frac{1}{\|g_{k+1}\|} + \frac{\|g_{k+1}\|}{g_{k+1}^T d_{k+1}} \right)^2 + \frac{1}{\|g_{k+1}\|^2} \\ &\leq \frac{\|d_k\|^2}{(g_k^T d_k)^2} + \frac{1}{\|g_{k+1}\|^2}. \end{aligned}$$

Because $\|d_1\|^2/(g_1^T d_1)^2 = 1/\|g_1\|^2$, (3.13) shows that

$$(3.14) \quad \frac{\|d_k\|^2}{(g_k^T d_k)^2} \leq \sum_{i=1}^k \frac{1}{\|g_i\|^2}$$

for all k . If the theorem is not true, there exists a constant $c > 0$ such that

$$(3.15) \quad \|g_k\| \geq c \quad \text{for all } k.$$

Therefore it follows from (3.14) and (3.15) that

$$(3.16) \quad \frac{\|d_k\|^2}{(g_k^T d_k)^2} \leq \frac{k}{c^2},$$

which implies that

$$(3.17) \quad \sum_{k \geq 1} \frac{(g_k^T d_k)^2}{\|d_k\|^2} = \infty.$$

Relation (3.17) contradicts the Zoutendijk condition (3.2). This contradiction shows that the theorem is true. \square

4. Discussion. It is shown in the previous section that the new conjugate gradient method converges under the standard Wolfe line search conditions. It should be noted that our assumption that the objective function is bounded below is weaker than the usual assumption that the level set

$$(4.1) \quad \{x \in \mathfrak{R}^n : f(x) \leq f(x_1)\}$$

is bounded.

From the proof of Theorem 3.3, we can see that the equivalent form (2.6) of the formula (2.4) plays an important role in the convergence analysis. Relation (2.6) enables us to establish the recurrence relation (3.13), which is about the sequence of the reciprocal $\{(g_k^T d_k)^2 / \|d_k\|^2\}$. The term $(g_k^T d_k)^2 / \|d_k\|^2$ is exactly the one that appears in the Zoutendijk condition (3.2). This makes our convergence analysis very simple. It is known that to obtain the convergence of the FR, PRP, and HS methods, one normally has to consider two sequences. For example, Al-Baali [1] considered the sequences $\{\|d_k\|^2\}$ and $\{g_k^T d_k / \|g_k\|^2\}$ for the FR method, and Gilbert and Nocedal [8] considered $\{\|d_k\|^2\}$ and $\{g_k^T d_k\}$ for the PRP and HS methods.

It is also worth noting that Al-Baali [1] and Gilbert and Nocedal [8] proved or required the sufficient descent condition, namely,

$$(4.2) \quad g_k^T d_k \leq -c \|g_k\|^2 \quad \text{for some } c > 0 \text{ and for all } k \geq 1.$$

However, our method does not guarantee this inequality. But if the strong Wolfe line search conditions are satisfied at every iteration, we have that

$$(4.3) \quad l_k = \frac{g_{k+1}^T d_k}{g_k^T d_k} \in [-\sigma, \sigma].$$

Formula (2.5) can be rewritten as

$$(4.4) \quad g_{k+1}^T d_{k+1} = \frac{1}{l_k - 1} \|g_{k+1}\|^2.$$

The above two relations show that (4.2) holds with $c = 1/(1 + \sigma)$. This indicates that our method also has the sufficient descent property (4.2) if the strong Wolfe line search conditions are used.

Dai and Yuan [3] considered a class of methods that use

$$(4.5) \quad \beta_k \in [(\sigma - 1)/(1 + \sigma), 1] \bar{\beta}_k,$$

where $\bar{\beta}_k$ is given by (2.4). It is shown in [3] that Algorithm 2.1 is still convergent if, in Step 4, β_k computed by (2.4) is replaced by any β_k , satisfying (4.5).

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