A new conjugate gradient method with the new Armijo search based on a modified secant equations

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ABSTRACT: It’s very effective for the conjugate gradient method to solve large-scale minimization problems. In this paper, based on the modified secant equations, we propose a new conjugate gradient method with the modified Armijo – type linear search. Under some proper conditions, the global convergence of this method is established.

KEYWORDS: unconstrained optimization problem; conjugate gradient method; secant equations; Armijo-type search; global convergence

I. INTRODUCTION

It is well known that the conjugate gradient method is an effective method to solve large-scale minimization problems ([3, 5, 7, 8, 9, 10]). The conjugate gradient method has a wide range of applications in many domains, like control science, engineering and operation research, etc.

The iterative formula of the conjugate gradient method is given as follows:

$$x_{k+1} = x_k + \alpha_k d_k, k = 0, 1, 2, \ldots,$$

where $\alpha_k$ denotes the step size, $d_k$ is defined by:

$$d_k = \begin{cases} -g_k, & k = 0, \\ -g_k + \beta_k d_{k-1}, & k \geq 1. \end{cases}$$

(1.2)

There are many formulae about $\beta_k$, see[1], for example, some famous formulae are defined as follows:

$$\beta_{k}^{FR} = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}, \quad \beta_{k}^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{\|g_{k-1}\|^2},$$

$$\beta_{k}^{HS} = \frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T (g_k - g_{k-1})}, \quad \beta_{k}^{LS} = -\frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T g_{k-1}}.$$  


Assume that the objective function $f$ is smooth sufficiently, we can make its Taylor expansion at point $x_{k-1} = x_k - s_{k-1}$. 


\[ f_{k-1} = f_k - s_k^T g_k + \frac{1}{2} s_k^T G_k s_k - \frac{1}{6} s_k^T (T_k s_k) s_k + O\left(\|s_{k-1}\|^4\right), \]
\[ s_k^T g_k = s_k^T g_k - s_k^T G_k s_k + \frac{1}{2} s_k^T (T_k s_k) s_k + O\left(\|s_{k-1}\|^4\right), \]
where
\[ s_k^T (T_k s_k) s_k = \sum_{i,j=1}^{n} \frac{\partial^3 f(x_k)}{\partial x_i \partial x_j \partial x_l} s_k^i s_k^j s_k^l. \]

This formula can be written as (see [14]):
\[ s_k^T G_s y_s = s_k^T y_s + \theta_{k-1}, \quad (1.3) \]
where \( \theta_{k-1} = 6(f_{k-1} - f_k) + 3(g_{k-1} - g_k)^T s_{k-1}, \)
\[ y_{k-1} = g_k - g_{k-1}. \]

Based on the formula (1.3), \( Y \) are Takano [15] considered the following extended secant equation:
\[ B_k s_{k-1} = Z_{k-1}, Z_{k-1} = y_{k-1} + \rho \frac{\theta_{k-1}}{s_{k-1}^T u}, \quad (1.4) \]
where \( u \in \mathbb{R}^n \) is any vector which satisfies \( s_{k-1}^T u \neq 0 \).

Generally speaking, based on the classical Armijo linear search technique, under some proper conditions, many conjugate gradient methods possess the descent property and the global convergence. But the drawback of the Armijo linear search is how to choose the initial step size. If it is too large, then more function evaluations are needed, if it is too small, then the efficiency of relevant algorithm will be decreased. In this paper, firstly, we modify the secant equation (1.4) and obtain a new secant equation, then present a new conjugate gradient method and propose a modified Armijo linear search technique which aims at the above drawback of Armijo linear search. Under some appropriate conditions, the global convergence is given for the new conjugate gradient method with the modified Armijo linear search.

II. NEW CONJUGATE GRADIENT METHOD

We propose the following modified secant equation
\[ B_k s_{k-1} = y_{k-1}, \]
\[ \bar{y}_{k-1} = y_{k-1} + \rho_{k-1} \frac{|\theta_{k-1}|}{s_{k-1}^T y_{k-1}} y_{k-1} + (1 - \rho_{k-1}) \frac{|\theta_{k-1}|}{s_{k-1}^T s_{k-1}} s_{k-1}, \quad (2.1) \]
Based on the above mentioned secant equation, a new formula of \( \beta_k \) is proposed:
\[ \beta_k = \begin{cases} 0, & \text{if } k = 1, \\ \frac{s_k^T y_{k-1} - t s_k^T s_{k-1}}{y_{k-2}^T d_{k-2}^2 ||d_{k-1}|| + \varepsilon ||d_{k-1}||^2}, & \text{if } k > 1, \end{cases} \quad (2.2) \]
where \( t \geq 0, \varepsilon > 0, \bar{y}_{k-1} \) is presented by (2.1).

The forthcoming proposition is clearly known in [13,14].
Proposition 2.1 \(|\theta_{k-1}| \leq 3L\|s_{k-1}\|^2\).

Definition 2.1 A twice continuously differentiable function \(f\) is uniformly convex on the nonempty open convex set \(S\) if and only if there exists \(M > 0\) such that
\[
(g(x) - g(y))^T (x - y) \geq M\|x - y\|^2, \quad \forall x, y \in S.
\]

In order to discuss the effectiveness of the conjugate gradient method (2.2), the following basic assumptions are given.

H 2.1 The objective function \(f(x)\) is continuously differentiable and has a lower bound on \(\mathbb{R}^n\).

H 2.2 The gradient \(g(x) = \nabla f(x)\) of function \(f(x)\) is Lipschitz continuously on the open convex set \(B\) with the level set \(L(x_0) = \{x \in \mathbb{R}^n \mid f(x) \leq f(x_0)\} (x_0 \text{ is given}), that is, there exists a constant \(L\) such that
\[
\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|, \forall x, y \in B.
\]

H 2.3 The level set \(L(x_0) = \{x \mid f(x) \leq f(x_0)\}\) has a bound, that is, there exists a constant \(C\) such that
\[
\|x\| \leq C, \forall x \in L(x_0).
\]

According to our modified secant equations, the following proposition is obtained clearly.

Proposition 2.2 \(\|y_{k-1}^*\| \leq \left(4 + \frac{3L}{M}\right)L\|s_{k-1}\|\).

Proof. By Definition 2.1, we have
\[
d^T_{k-1}y_{k-1}^* \geq \left(1 + \rho_{k-1}\frac{|\theta_{k-1}|}{\|s_{k-1}\|}\right)d^T_{k-1}y_{k-1} \geq d^T_{k-1}y_{k-1} \geq M\alpha^{-1}_{k-1}\|s_{k-1}\|^2. \quad (2.5)
\]

Considering (2.1), if the assumptions H 2.2 and H 2.3 hold, and \(\rho_{k-1} \in [0,1]\), we have
\[
\|y_{k-1}^*\| \leq \|y_{k-1}\| + \rho_{k-1}\frac{|\theta_{k-1}|}{\|s_{k-1}\|}\|s_{k-1}\| + (1 - \rho_{k-1})\frac{|\theta_{k-1}|}{\|s_{k-1}\|}\|s_{k-1}\|
\leq L\|s_{k-1}\| + \frac{3L\|s_{k-1}\|^2}{M}\|y_{k-1}\| + \frac{3L\|s_{k-1}\|^2}{\|s_{k-1}\|^2}\|s_{k-1}\|
\leq \left(4 + \frac{3L}{M}\right)L\|s_{k-1}\|.
\]

Recently, some methods to obtain the Lipschitz constant \(L\) were proposed [11,12]. If \(k \geq 1\), let \(y_{k-1} = g_k - g_{k-1}\), the following three estimating formulae were obtained
\[
L \left\| \frac{y_{k-1}}{s_{k-1}} \right\| \quad (2.6)
\]
In fact, any scalar which is greater than $L$ can be regarded as a *Lipschitz* constant, however it is possible to cause the slow convergence rate. So it is very important to find the *Lipschitz* constant which is as small as possible and is effective for practical computation.

In the $k$th iteration we take respectively the *Lipschitz* constant as:

\[
L_k = \max \left( L_{k-1}, \frac{\|y_{k-1}\|}{\|s_{k-1}\|} \right),
\]

(2.9)

\[
L_k = \max \left( L_{k-1}, \min \left( \frac{\|y_{k-1}\|^2}{s_{k-1}^T y_{k-1}}, M_0^\alpha \right) \right),
\]

(2.10)

\[
L_k = \max \left( L_{k-1}, \frac{s_{k-1}^T y_{k-1}}{\|s_{k-1}\|^2} \right),
\]

(2.11)

where $L_0 > 0$ and $M_0^\alpha$ is a large positive number. Corresponding to the three *Lipschitz* constants, we call the conjugate method as $A1, A2, A3$ respectively.

Now, based on [1], we present the following modified *Armijo* linear search:

Given $\mu \in \left( 0, \frac{1}{2} \right)$, $\rho \in (0, 1)$, $c \in (0, 1)$, $\varepsilon \in (0, 1)$,

let

\[
l_k = \frac{1 - c}{\theta_0} y_{k-1}^T d_{k-1} + \varepsilon \|d_k\|, \quad \theta_0 = 4L_k + \frac{3L_k^2}{M} + t,
\]

where $t$ is mentioned in (2.1), $M$ is defined in Definition 2.1, and $\alpha_k$ is the largest $\alpha$ which belongs to $\left\{ l_k, l_k \rho, l_k \rho^2, \ldots \right\}$ satisfying:

\[
f_k - f(x_k + \alpha d_k) \geq -\alpha \mu g_k^T d_k,
\]

while $L_k$ is given in (2.9), (2.10), and (2.11), respectively.

Based on the modified *Armijo* linear search and the new formula of $\beta_k$, we propose the following modified conjugate gradient algorithm.

**Algorithm:**

*Step 0* Choose $x_0 \in R^n$, set $d_0 = -g_0, k = 0$.

*Step 1* if $\|g_k\| = 0$, stop, otherwise go to Step 2.

*Step 2* Let $x_{k+1} = x_k + \alpha_k d_k$, where $d_k$ is followed by (1.2), $\beta_k$ is defined by (2.2), and $\alpha_k$ is defined by the
modified Armijo – type linear search.

Step 3 Let $k := k + 1$, go back to step 1.

III. GLOBAL CONVERGENCE OF THE ALGORITHM

Lemma 3.1 Suppose that $H \ 2.1$ and $H \ 2.2$ hold, and the new conjugate gradient method with the modified Armijo – type linear search generates an infinite sequence $\{x_k\}$, then there exist the constant $m_0$ and $M_0$ such that $m_0 < L_k < M_0$.

Lemma 3.2 Suppose that $H \ 2.1$ and $H \ 2.2$ hold, the new conjugate gradient method with the new Armijo – type linear search generates an infinite sequence $\{x_k\}$. Then for $k \geq 1$,

$$
\alpha_k \leq \frac{1-c}{\theta} \left| y_{k-1}^T d_{k-1} \right| + \varepsilon \|d_k\|
$$

where $\theta = 4L + \frac{3L^2}{M} + t$, we have

$$
g_{k+1}^T d_{k+1} \leq -c \|g(x_{k+1})\|^2.
$$

Proof. By the Cauchy–Schwarz inequality, we have

$$
(1-c)\left| y_{k-1}^T d_{k-1} \right| + \varepsilon \|d_k\| \geq \alpha_k \|d_k\|
$$

$$
= \frac{\alpha_k \theta \cdot \|d_k\|^2 \left( \left| y_{k-1}^T d_{k-1} \right| + \varepsilon \|d_k\| \right)}{\left| y_{k-1}^T d_{k-1} \right| \|d_k\| + \varepsilon \|d_k\|^2} \cdot \|g_{k+1}\|^2
$$

$$
\geq \frac{\alpha_k \theta \|g_{k+1}\| \|d_k\|}{\left| y_{k-1}^T d_{k-1} \right| \|d_k\| + \varepsilon \|d_k\|^2} \cdot \left| y_{k-1}^T d_{k-1} + \varepsilon \|d_k\| \right| \cdot g_{k+1}^T d_k
$$

thereby, we know that

$$
\left| g_{k+1}^T y_k - t g_{k+1}^T s_k \right| \leq \|g_{k+1}\| \left| y_k \right| + t \|g_{k+1}\| \|s_k\|
$$

$$
\leq \|g_{k+1}\| \left( 4L + \frac{3L^2}{M} + t \right) \alpha_k \|d_k\|
$$

$$
= \alpha_k \theta \|g_{k+1}\| \|d_k\|
$$

so
(1−c)||yk−1Td−k−1|| + ε ||d_k|| ≥ \begin{align*}
& \frac{||g_{k+1}^Ty_k - t g_k^Ts_k||}{||y_{k-1}^Td_{k-1}|| + \varepsilon ||d_{k-1}||} \cdot \frac{||g_{k+1}^Td_k||}{||s_{k+1}||} \\
& \geq \beta_{k+1} \left(\frac{||y_{k-1}^Td_{k-1} + \varepsilon ||d_k||}{||s_{k+1}||} \right) g_{k+1}^Td_k
\end{align*}

thus

(1−c)||g_{k+1}||^2 ≥ \beta_{k+1} g_{k+1}^Td_k

that is,

−c||g_{k+1}||^2 ≥ −||g_{k+1}||^2 + \beta_{k+1} g_{k+1}^Td_k = g_{k+1}^Td_{k+1}.

The proof is completed.

**Lemma 3.3** Suppose that H 2.1 and H 2.2 hold, the new conjugate gradient method with the new Armijo – type linear search generates an infinite sequence {x_k}, then ||d_k|| ≤ (2−c)||g_k|| ∀k, where m_0 is defined in Lemma 3.1.

Proof. When k = 0 or 1, ||d_k|| = ||g_k|| ≤ (2−c)||g_k||.

For k > 1, we have

||d_k|| = ||−g_k + \beta_k d_{k−1}||

≤ ||g_k|| + \left|\frac{g_{k+1}^Ty_{k−1} - t g_k^Ts_{k−1}}{||y_{k−2}^Td_{k−2}|| + \varepsilon ||d_{k−1}||} \right| ||d_{k−1}||

≤ ||g_k|| + \alpha_{k−1} \theta ||g_k|| ||d_{k−1}||

≤ (2−c)||g_k||.

The proof is completed.

**Lemma 3.4** Suppose that H 2.1 and H 2.2 hold, then the modified Armijo – type linear search is well-defined.

Proof. When \alpha_k = \frac{1−c||y_{k−1}^Td_{k−1} + \varepsilon ||d_{k−1}||}{\theta_0 ||d_{k−1}||}, we have that

\alpha_k = \frac{1−c||y_{k−1}^Td_{k−1} + \varepsilon ||d_{k−1}||}{\theta_0 ||d_{k−1}||} \geq \frac{1−c}{\theta_0} \varepsilon.
When \( \alpha_k < \frac{1 - c}{\theta_0} \left\| y^T_{k-1} d_{k-1} + \varepsilon \right\| d_k \), for \( \alpha = \rho^{-1} \alpha_k \), we have the following inequality:

\[
f_k - f(x_k + \alpha d_k) < -\alpha \mu g^T_k d_k.
\]

Using the Mean Value Theorem on the left-hand side of the above inequality, there exists a scalar \( t_k \in (0,1) \) such that,

\[
-\alpha g \left( x_k + t_k \alpha d_k \right)^T d_k < -\alpha \mu g^T_k d_k,
\]

that is,

\[
g \left( x_k + t_k \alpha d_k \right)^T d_k > \mu g^T_k d_k.
\]

By the condition \( H2 \), according to the Cauchy - Schwarz inequality and Lemma 3.1, it holds that

\[
L \|d_k\|^2 \geq \|g \left( x_k + t_k \alpha d_k \right) - g_k\|d_k\|
\]

\[
\geq g \left( x_k + t_k \alpha d_k \right)^T d_k
\]

\[
\geq (1 - \mu) g^T_k d_k
\]

\[
\geq c(1 - \mu) \|g_k\|^2,
\]

i.e.

\[
\alpha_k \geq \frac{c \rho (1 - \mu) \|g_k\|^2}{\|d_k\|^2} \geq \frac{c \rho (1 - \mu)}{L(2 - c)^2}.
\]

So there exists \( \alpha_k \geq \min \left\{ \frac{1 - c}{\theta_0} \varepsilon, \frac{c \rho (1 - \mu)}{L(2 - c)^2} \right\} \) such that the modified Armijo - type linear search is well-defined.

The proof is completed.

Theorem 3.1 Suppose that \( H2.1 \) and \( H2.2 \) hold, the new conjugate gradient method with the new Armijo - type linear search generates an infinite sequence \( \{x_k\} \). Then \( \lim_{k \to \infty} \|g_k\| = 0. \)

Proof. Let \( \eta_0 = \inf \left\{ \alpha_k \right\} \), if \( \eta_0 > 0 \), then

\[
f_k - f \left( x_k + \alpha d_k \right) \geq -\alpha \mu g^T_k d_k \geq \mu \eta_0 c \|g_k\|^2.
\]

By the condition \( H2.1 \), we have \( \sum_{k=0}^{+\infty} \|g_k\|^2 < +\infty \), so it holds that

\[
\lim_{k \to \infty} \|g_k\| = 0.
\]

By the contrary, suppose that \( \eta_0 = 0 \). Then there exists an infinite subset \( K \subseteq \{0,1,2,\ldots\} \) such that
\[
\lim_{k \in K, x \to \infty} \alpha_k = 0. \\
\text{(3.1)}
\]

By Lemma 3.1 and Lemma 3.4, we know that
\[
l_k = \frac{1 - c}{\theta_0} \left| y_{k-1}^T d_{k-1} \right| + \varepsilon \left\| d_k \right\| > \frac{(1 - c) \varepsilon}{\theta_0} > 0.
\]

From (3.1) there exists \( k' \) such that \( \rho^{-1} a_k \leq l_k \), \( \forall k \geq k', k \in K \).

Let \( \alpha = \rho^{-1} a_k \), it is obvious that
\[
f_k - f(x_k + a d_k) < -\alpha \mu g_k^T d_k.
\]

By the proof of Lemma 3.4, we have that
\[
L \alpha \left\| d_k \right\|^2 \geq c (1 - \mu) \left\| g_k \right\|^2.
\]

Then by Lemma 3.3, it holds that
\[
\alpha_k \geq \frac{c \rho (1 - \mu) \left\| g_k \right\|^2}{L \left\| d_k \right\|^2} \geq \frac{c \rho (1 - \mu)}{L} (2 - c)^{-2} > 0, k > k', k \in K.
\]

Which contradicts with (3.1). The proof is completed.

\[\text{IV. NUMERICAL EXPERIMENTS}\]

In this section, we carry out some numerical experiments. Our algorithm has been tested on some problems as follows, where \( x_0 \) is the initial point, and \( x_k \) is the final point.

Example 1. \( f(x) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \).

Example 2. \( f(x) = (x_2 - 1)^2 + (x_1 - 5)^2 \).

Example 3. \( f(x) = (x_1 - 2)^2 + (x_2 - 1)^2 + \frac{0.04}{(x_1^2/4 - x_2^2/3 + 1)^2} + \frac{0.004}{(x_1 - 2x_2 + 1)^2}. \)

We set the parameters \( \delta = 0.25, \rho = 0.5, c = 0.75 \) and \( L = 1 \) in the numerical experiment. The numerical results are given in Table 1.

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<th>( x_k )</th>
<th>k</th>
<th>time(s)</th>
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V. CONCLUSION

Table 1 shows the performance of the algorithm about relative to the iteration. It is easy to see that, for above problems, the algorithm is efficient. In particular, when the precision is not very strict, results for each problem are basically correct, and with less number of times of iteration.

REFERENCES