



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:

$$x_{k+1} = x_k + \alpha_k d_k, k = 0, 1, 2, \dots, \quad (1.1)$$

where α_k denotes the step size, d_k is defined by:

$$d_k = \begin{cases} -g_k, & k = 0, \\ -g_k + \beta_k d_{k-1}, & k \geq 1, \end{cases} \quad (1.2)$$

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

$$\beta_k^{FR} = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}, \quad \beta_k^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{\|g_{k-1}\|^2},$$
$$\beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T (g_k - g_{k-1})}, \quad \beta_k^{LS} = -\frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T g_{k-1}}.$$

Recently, [13] and [14] proposed a new secant equation.

Assume that the objective function f is smooth sufficiently, we can make its Taylor expansion at point

$$x_{k-1} = x_k - s_{k-1}.$$

$$f_{k-1} = f_k - s_{k-1}^T g_k + \frac{1}{2} s_{k-1}^T G_k s_{k-1} - \frac{1}{6} s_{k-1}^T (T_k s_{k-1}) s_{k-1} + O(\|s_{k-1}\|^4),$$

$$s_{k-1}^T g_{k-1} = s_{k-1}^T g_k - s_{k-1}^T G_k s_{k-1} + \frac{1}{2} s_{k-1}^T (T_k s_{k-1}) s_{k-1} + O(\|s_{k-1}\|^4),$$

where

$$s_{k-1}^T (T_k s_{k-1}) s_{k-1} = \sum_{i,j,l=1}^n \frac{\partial^3 f(x_k)}{\partial x^i \partial x^j \partial x^l} s_{k-1}^i s_{k-1}^j s_{k-1}^l.$$

This formula can be written as (see[14]):

$$s_{k-1}^T G_k s_{k-1} = s_{k-1}^T y_{k-1} + \theta_{k-1}, \tag{1.3}$$

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* and *Takano* [15] considered the following extended secant equation :

$$B_k s_{k-1} = Z_{k-1}, Z_{k-1} = y_{k-1} + \rho \frac{\theta_{k-1}}{s_{k-1}^T u} u, \tag{1.4}$$

where $u \in R^n$ 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

$$B_k s_{k-1} = y_{k-1}^*,$$

$$y_{k-1}^* = y_{k-1} + \rho_{k-1} \frac{|\theta_{k-1}|}{s_{k-1}^T y_{k-1}} y_{k-1} + (1 - \rho_{k-1}) \frac{|\theta_{k-1}|}{s_{k-1}^T s_{k-1}} s_{k-1}, \tag{2.1}$$

Based on the above mentioned secant equation, a new formula of β_k is proposed:

$$\beta_k = \begin{cases} 0, & \text{if } k = 1, \\ \frac{g_k^T y_{k-1}^* - t g_k^T s_{k-1}}{\|y_{k-2}^T d_{k-2}\| \|d_{k-1}\| + \varepsilon \|d_{k-1}\|^2}, & \text{if } k > 1, \end{cases} \tag{2.2}$$

where $t \geq 0, \varepsilon > 0, y_{k-1}^*$ 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 2.1A 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

$$(g(x) - g(y))^T (x - y) \geq M \|x - y\|^2, \forall x, y \in S.$$

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 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 $L(x_0) = \{x \in R^n | f(x) \leq f(x_0)\}$ (x_0 is given), that is, there exists a constant L such that

$$\|\nabla f(x) - \nabla f(y)\| \leq L \|x - y\|, \forall x, y \in B. \tag{2.3}$$

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

$$\|x\| \leq C, \forall x \in L(x_0). \tag{2.4}$$

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

$$d_{k-1}^T \overline{y_{k-1}^{*-}} \geq \left(1 + \rho_{k-1} \frac{|\theta_{k-1}|}{|s_{k-1}^T y_{k-1}|}\right) d_{k-1}^T y_{k-1} \geq d_{k-1}^T y_{k-1} \geq M \alpha_{k-1}^{-1} \|s_{k-1}\|^2. \tag{2.5}$$

Considering (2.1), if the assumptions **H2.2** and **H2.3** hold, and $\rho_{k-1} \in [0,1]$, we have

$$\begin{aligned} \|y_{k-1}^{*-}\| &\leq \|y_{k-1}\| + \rho_{k-1} \frac{|\theta_{k-1}|}{|s_{k-1}^T y_{k-1}|} \|y_{k-1}\| + (1 - \rho_{k-1}) \frac{|\theta_{k-1}|}{|s_{k-1}^T s_{k-1}|} \|s_{k-1}\| \\ &\leq L \|s_{k-1}\| + \frac{3L \|s_{k-1}\|^2}{M \|s_{k-1}\|^2} \|y_{k-1}\| + \frac{3L \|s_{k-1}\|^2}{\|s_{k-1}\|^2} \|s_{k-1}\| \\ &\leq \left(4 + \frac{3L}{M}\right) L \|s_{k-1}\|. \end{aligned}$$

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

$$L \square \frac{\|y_{k-1}\|}{\|s_{k-1}\|} \tag{2.6}$$

$$L \square \frac{\|y_{k-1}\|^2}{s_{k-1}^T y_{k-1}} \tag{2.7}$$

$$L \square \frac{s_{k-1}^T y_{k-1}}{\|s_{k-1}\|^2}, \tag{2.8}$$

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:

$$L_k = \max \left(L_{k-1}, \frac{\|y_{k-1}\|}{\|s_{k-1}\|} \right), \tag{2.9}$$

$$L_k = \max \left(L_{k-1}, \min \left(\frac{\|y_{k-1}\|^2}{s_{k-1}^T y_{k-1}}, M_0' \right) \right), \tag{2.10}$$

$$L_k = \max \left(L_{k-1}, \frac{s_{k-1}^T y_{k-1}}{\|s_{k-1}\|^2} \right), \tag{2.11}$$

where $L_0 > 0$ and M_0' 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 $l_k = \frac{1-c}{\theta_0} \frac{|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|}{\|d_k\|}$, $\theta_0 = 4L_k + \frac{3L_k^2}{M} + t$, where t is mentioned in (2.1), M is defined in

Definition 2.1, and α_k is the largest α which belongs to $\{l_k, l_k \rho, l_k \rho^2, \dots\}$ 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 β_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), β_k is defined by (2.2), and α_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 $k \geq 1$,

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

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

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

thereby, we know that

$$\begin{aligned} \left| g_{k+1}^T \bar{y}_k - t g_{k+1}^T s_k \right| &\leq \|g_{k+1}\| \left\| \bar{y}_k \right\| + t \|g_{k+1}\| \|s_k\| \\ &\leq \|g_{k+1}\| \left(4L + \frac{3L^2}{M} + t \right) \alpha_k \|d_k\| \\ &= \alpha_k \theta \|g_{k+1}\| \|d_k\|, \end{aligned}$$

so

$$(1-c)(|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|) \geq \frac{|g_{k+1}^T \bar{y}_k - t g_{k+1}^T s_k|}{(|y_{k-1}^T d_{k-1}| \|d_k\| + \varepsilon \|d_k\|^2)} \cdot \frac{(|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|) \cdot g_{k+1}^T d_k}{\|g_{k+1}\|^2}$$

$$\geq \beta_{k+1} \frac{(|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|) g_{k+1}^T d_k}{\|g_{k+1}\|^2}$$

thus

$$(1-c) \|g_{k+1}\|^2 \geq \beta_{k+1} g_{k+1}^T d_k$$

that is,

$$-c \|g_{k+1}\|^2 \geq -\|g_{k+1}\|^2 + \beta_{k+1} g_{k+1}^T d_k = g_{k+1}^T d_k.$$

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 $\|d_k\| \leq (2-c) \|g_k\|, \forall k$, where m_0 is defined in Lemma 3.1.

Proof. When $k = 0$ or 1 , $\|d_k\| = \|g_k\| \leq (2-c) \|g_k\|$.

For $k > 1$, we have

$$\|d_k\| = \|-g_k + \beta_k d_{k-1}\|$$

$$\leq \|g_k\| + \frac{|g_k^T \bar{y}_{k-1} - t g_k^T s_{k-1}|}{|y_{k-2}^T d_{k-2}| \|d_{k-1}\| + \varepsilon \|d_{k-1}\|^2} \|d_{k-1}\|$$

$$\leq \|g_k\| + \frac{\alpha_{k-1} \theta \|g_k\| \|d_{k-1}\|}{|y_{k-2}^T d_{k-2}| + \varepsilon \|d_{k-1}\|}$$

$$\leq (2-c) \|g_k\|.$$

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 $\alpha_k = \frac{1-c}{\theta_0} \frac{|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|}{\|d_k\|}$, we have that

$$\alpha_k = \frac{1-c}{\theta_0} \frac{|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|}{\|d_k\|} \geq \frac{1-c}{\theta_0} \varepsilon.$$

When $\alpha_k < \frac{1-c}{\theta_0} \frac{|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|}{\|d_k\|}$, for $\alpha = \rho^{-1} \alpha_k$, we have the following inequality:

$$f_k - f(x_k + \alpha d_k) < -\alpha \mu g_k^T d_k.$$

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,

$$-\alpha g(x_k + t_k \alpha d_k)^T d_k < -\alpha \mu g_k^T d_k,$$

that is,

$$g(x_k + t_k \alpha d_k)^T d_k > \mu g_k^T d_k.$$

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

$$\begin{aligned} L\alpha \|d_k\|^2 &\geq \|g(x_k + t_k \alpha d_k) - g_k\| \|d_k\| \\ &\geq g(x_k + t_k \alpha d_k)^T d_k \\ &\geq -(1-\mu) g_k^T d_k \\ &\geq c(1-\mu) \|g_k\|^2, \end{aligned}$$

i.e.

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

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 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 $\lim_{k \rightarrow \infty} \|g_k\| = 0$.

Proof. Let $\eta_0 = \inf_{\forall k} \{\alpha_k\}$, if $\eta_0 > 0$, then

$$f_k - f(x_k + \alpha d_k) \geq -\alpha \mu g_k^T d_k \geq \mu \eta_0 c \|g_k\|^2.$$

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

$$\lim_{k \rightarrow \infty} \|g_k\| = 0.$$

By the contrary, suppose that $\eta_0 = 0$. Then there exists an infinite subset $K \subseteq \{0,1,2,\dots\}$ such that

$$\lim_{k \in K, x \rightarrow \infty} \alpha_k = 0. \tag{3.1}$$

By Lemma 3.1 and Lemma 3.4, we know that

$$l_k = \frac{1-c}{\theta_0} \frac{|y_{k-1}^T d_{k-1}| + \varepsilon \|d_k\|}{\|d_k\|} > \frac{(1-c)\varepsilon}{\theta_0} > 0.$$

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

Let $\alpha = \rho^{-1} \alpha_k$, it is obvious that

$$f_k - f(x_k + \alpha d_k) < -\alpha \mu g_k^T d_k.$$

By the proof of Lemma 3.4, we have that

$$L \alpha \|d_k\|^2 \geq c(1-\mu) \|g_k\|^2.$$

Then by Lemma 3.3, it holds that

$$\alpha_k \geq \frac{c\rho(1-\mu)}{L} \frac{\|g_k\|^2}{\|d_k\|^2} \geq \frac{c\rho(1-\mu)}{L} (2-c)^{-2} > 0, k > k', k \in K.$$

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

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. $f(x) = (x_1 - 2)^2 + (x_2 - 1)^2 + \frac{0.04}{(-x_1^2/4 - x_2^2 + 1)} + \frac{(x_1 - 2x_2 + 1)^2}{0.2}$.

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.

Table 1:

NO.	eps	x_0	x_k	k	time(s)
1	10e-3	(4, 4)	(2.9999, 2.0004)	29	0.008384
1	10e-2	(4, 4)	(2.9992, 2.0011)	8	0.002126
2	10e-3	(2, -1)	(4.9958, 0.9972)	414	0.074989
2	10e-2	(2, -1)	(4.9588, 0.9725)	43	0.005031
3	10e-3	(2, 1)	(1.8000, 1.3802)	219	0.026329
3	10e-2	(2, 1)	(1.8061, 1.3817)	3	0.026329



ISSN: 2350-0328

International Journal of Advanced Research in Science, Engineering and Technology

Vol. 5, Issue 7 , July 2018

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.

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