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An Extended Spectral Conjugate Gradient Method for Unconstrained Optimization Problems

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Author's contributions

This work was carried out in collaboration between all authors. All authors read and approved the final manuscript.

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Abstract

In this paper, an extended spectral conjugate gradient method is proposed for solving unconstrained optimization problems, where the search direction is a linear combination of the gradient vector at current iteration and the search direction at the previous iteration. Instead of specifying a fixed expression to compute each combination coefficient in the existent methods, only suitable conditions are presented for the combination coefficients such that the values of coefficients are chosen freely in a range. Under some mild assumptions, with step lengths satisfying the Armijo condition, global convergence is established for the developed algorithm. It is shown that some existent methods are the special cases of the presented method in this paper.

Keywords: *Unconstrained optimization; conjugate gradient method; line search; global convergence.*

AMS Subject Classification (2010): 90C25, 90C30.

1 Introduction

Consider the following unconstrained optimization problem:

$$\min f(x), x \in R^n, \qquad (1)$$

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where $f : R^n \to R$ is a continuously differentiable objective function. Amongst all existent solution methods for solving (1), nonlinear conjugate gradient method is paid a lot of attentions recently owing to the simplicity of computation and the requirement of low memory. In this connection, one can see, for example,[1-14] and the references therein.

As an extension of the ordinary conjugate gradient methods, spectral conjugate gradient method is often more efficient in numerical performance than the others since it incorporates the advantages of spectral method and conjugate gradient method into constructing a search direction. For recent advancement his aspect, see, for example, [3,6,8,10-14].

Different from the existent spectral conjugate gradient methods, where the search direction is a linear combination of the gradient vector at current iteration and the search direction at the previous iteration, in this paper, we intend to investigate an extended spectral conjugate gradient method for solving unconstrained optimization problems. Instead of specifying a fixed expression to compute each combination coefficient in the existent methods, only suitable conditions are presented for the combination coefficients such that the values of coefficients are chosen freely in a range. Thus, the proposed method in this paper is an extended version of spectral conjugate gradient method. Under some mild assumptions, with step lengths satisfying the Armijo condition, we will establish global convergence for the developed algorithm. To show the generalization of the method, some existent methods will be proved to be its special cases.

The rest of this paper is organized as follows. In next section, a generic framework of spectral conjugate gradient method is presented. Some sufficient conditions are given to establish the global convergence in Section 3. In Section 4, it is shown that several existing methods are the special cases of our method. Some final remarks are given in the last section.

2 Generic Framework of the Developed Method

In the classical conjugate gradient method, a search direction d_k at the current iterate point x_k is determined by

$$d_k = \begin{cases} -g_0, & if \quad k = 0, \\ -g_k + \beta_k d_{k-1}, & if \quad k \geq 1, \end{cases} \tag{2}$$

Where β_k is called the conjugacy coefficient, g_k is the value of the gradient function g at x_k.

Different from the classical conjugate gradient method, in a spectral conjugate gradient method, the search direction d_k is defined as follows:

$$d_k = \begin{cases} -g_0, & if \quad k = 0, \\ -\theta_k g_k + \beta_k d_{k-1}, & if \quad k \geq 1, \end{cases} \tag{3}$$

where θ_k is called a spectral coefficient. It is easy to see that (3) reduces to (2) if $\theta_k = 1$. Since there are two types of parameters can be suitably chosen to obtain a search direction in (3), it is possible that (3) combines the advantages of spectral method and conjugate gradient method.

However up to now, in the existent methods, it is by specifying a fixed expression for the spectral coefficient and the conjugacy coefficient in (2) or (3) such that a desired search direction d_k is obtained to improve the efficiency of algorithm and establish the convergence. Instead, in this paper, we are going to present an extended spectral conjugate gradient method, which allows the spectral coefficient and the conjugacy coefficient to be chosen freely in a range defined by some suitable conditions (see Assumption 2 in Section 3). In addition, we extend (3) to the following more generic form:

$$d_k = \begin{cases} -g_0 & \text{if} \quad k = 0, \\ D(g_k, g_{k-1}, \ldots, g_{k-l_1}, d_{k-1}, d_{k-2}, \ldots, d_{k-1-l_2}) & \text{if} \quad k \geq 1, \end{cases} \tag{4}$$

where $D : R^{l_1+l_2+2} \to R^n$ is a vector-value function, it is called the **direction function**, $0 \leq l_1 \leq k$ and $0 \leq l_2 \leq k-1$. If $l_1 = 0$, $l_2 = 0$ and D is linear, then (4) reduces (3).

Remark 1: *In the generalized spectral conjugate gradient method (4), to obtain a suitable search direction d_k, the direction function D should owns some properties such that the performance of the corresponding algorithm is improved. In particular, if D is a linear combination of the vectors g_k, $g_{k-1}, \ldots, g_{k-l_1}$, $d_{k-1}, d_{k-2}, \ldots, d_{k-1-l_2}$, then the choices of combination coefficients play an important role in the design of efficient algorithm and in the establishment of convergence. It really is an interesting issue to specify analytic expression to compute all the coefficients or to present some suitable conditions for these coefficients, but we focus on presenting suitable conditions on the coefficients in (3) for convenience of establishing the global convergence for the developed algorithm.*

In the end of this section, we state a framework of the extended spectral conjugate gradient algorithm as follows.

Algorithm 1:

Step 0. Choose a tolerant constant $\varepsilon > 0$. Choose an initial point $x_0 \in R^n$. Let $k := 0$.

Step 1. If $\|g_k\| \leq \varepsilon$, then the algorithm stops. Otherwise, compute d_k by (4). Go to Step 2.

Step 2. Determine a step length α_k by a line search strategy.

Step 3. Set $x_{k+1} := x_k + \alpha_k d_k$, and $k := k+1$. Return to Step 1.

3 Global Convergence

In this section, we are going to find some conditions which ensure the global convergence of Algorithm 1. For sake of simplicity, it is studied for the case that $l_1 = 0$, $l_2 = 0$ and D is linear in (4), which is defined as in (3).

We first give two mild assumptions on the structure of Problem (1).

Assumption 1:
(1) The level set $\Omega = \{x \in R^n \mid f(x) \le f(x_0)\}$ is bounded for a given initial point x_0.
(2) In some neighborhood N of Ω, f is continuously differentiable and its gradient is Lipschitz continuous. It says that there exists a constant $L > 0$ such that

$$\|g(x) - g(y)\| \le L\|x - y\|, \forall\ x, y \in N \tag{5}$$

The following conditions are on the direction and the step length generated by Algorithm 1.

Assumption 2:
(1) (a) For $k \ge 0$, we have

$$g_k^T d_k = -\|g_k\|^2 \tag{6}$$

(b) For $k \ge 0$, the inequality

$$|\beta_k| \le \frac{\|g_k\|^2}{\|g_{k-1}\|^2} \tag{7}$$

holds.
(2) For $k \ge 0$, define

$$\alpha_k = c_k \tilde{\alpha}_k \tag{8}$$

where $\tilde{\alpha}_k$ is a step length satisfying:

$$f(x_k + \alpha_k d_k) \le f(x_k) + \delta \alpha_k g_k^T d_k \tag{9}$$

with a constant $\delta \in (0,1)$. For such an α_k, suppose that $\{c_k\}$ is bounded.

Remark 2: It is noted that Assumption 2(1) is on the search direction, and Assumption 2(2) on the step length.

Before stating a theorem of global convergence, we first prove the following lemma.

Lemma 1: Under Assumptions 1 and 2, it is obtained that

$$\sum_{k\geq 0}\frac{\|g_k\|^4}{\|d_k\|^2}<\infty \tag{10}$$

Proof: From the Armijo line search rule, we know that $\rho^{-1}\alpha_k$ satisfies the following inequality

$$f(x_k+\rho^{-1}\alpha_k d_k)-f(x_k)>\sigma_1\alpha_k\rho^{-1}g_k^T d_k \tag{11}$$

From Assumption 1(2), we have

$$\begin{aligned}f\left(x_k+\rho^{-1}\alpha_k d_k\right)-f\left(x_k\right)&=\rho^{-1}\alpha_k g\left(x_k+t_k\rho^{-1}\alpha_k d_k\right)^T d_k\\&=\rho^{-1}\alpha_k g_k^T d_k+\rho^{-1}\alpha_k\left(g\left(x_k+t_k\rho^{-1}\alpha_k d_k\right)-g_k\right)^T d_k\\&\leq\rho^{-1}\alpha_k g_k^T d_k+L\rho^{-2}\alpha_k^2\|d_k\|^2.\end{aligned}$$

where $t_k\in(0,1)$ is a constant scalar such that $x_k+t_k\rho^{-1}\alpha_k\in\Omega$.

Therefore, from (11), it is obtained that

$$\sigma_1\alpha_k\rho^{-1}g_k^T d_k<\rho^{-1}\alpha_k g_k^T d_k+L\rho^{-2}\alpha_k^2\|d_k\|^2$$

It reads

$$(1-\sigma_1)\alpha_k g_k^T d_k+L\rho^{-2}\alpha_k^2\|d_k\|^2>0$$

From (6), it follows that

$$\alpha_k>\frac{\rho(1-\sigma_1)\|g_k\|^2}{L\|d_k\|^2}$$

Taking

$$m=\frac{\rho\left(1-\sigma_1\right)}{L}.$$

Then, from the line search rule (8) and Assumption 1, it follows that there exists a constant M such that

$$\begin{aligned}\sum_{k=0}^{n-1}\left(-\sigma_1 a_k g_k^T d_k\right)&=\sum_{k=0}^{n-1}\left(-\sigma_1 c_k\alpha_k g_k^T d_k\right)\\&\leq\sum_{k=0}^{n-1}\left(-\sigma_1 c_1\alpha_k g_k^T d_k\right)\\&\leq c_1\sum_{k=0}^{n-1}\left(f\left(x_k\right)-f\left(x_k+1\right)\right)\end{aligned}$$

$$= c_1 \left[f(x_0) - f(x_n) \right] < 2c_1 M$$

where $c_1 = \max\{c_k\}$.

Combined with (6), we have

$$\begin{aligned} 2c_1 M &> \sum_{k=0}^{n-1} \left(-\sigma_1 \alpha_k g_k^T d_k \right) \\ &= \sum_{k=0}^{n-1} (\sigma_1 \alpha_k \|g_k\|^2) = \sum_{k=0}^{n-1} (\sigma_1 c_k \bar{\alpha}_k \|g_k\|^2) \\ &\geq \sum_{k=0}^{n-1} (\sigma_1 \mu c_2 \frac{\|g_k\|^4}{\|d_k\|^2}) \end{aligned}$$

where $c_2 = \min\{c_k\}$.The desired result is obtained.

Now, we are in a position to present the main theorem in this paper.

Theorem 1: Let $\{x_k\}$ be a sequence generated by Algorithm 1.Under Assumptions 1 and 2, the following result holds:

$$\lim_{k \to \infty} \inf \|g_k\| = 0. \qquad (12)$$

Proof : Suppose that there exists a positive constant $\varepsilon > 0$ such that

$$\|g_k\| \geq \varepsilon \qquad (13)$$

for all k. Then, from (3), it follows that

$$\begin{aligned} \|d_k\|^2 &= d_k^T d_k \\ &= \left(-\theta_k g_k^T + \beta_k d_{k-1}^T \right)\left(-\theta_k g_k + \beta_k d_{k-1} \right) \\ &= \theta_k^2 \|g_k\|^2 - 2\theta_k \left(d_k^T + \theta_k g_k^T \right) g_k + \left(\beta_k \right)^2 \|d_{k-1}\|^2 \\ &= \theta_k^2 \| g_k \|^2 - 2\theta_k d_k^T g_k - 2\theta_k^2 \| g_k \|^2 + (\beta_k)^2 \| d_{k-1} \|^2 \\ &= (\beta_k)^2 \| d_{k-1} \|^2 - 2\theta_k d_k^T g_k - \theta_k^2 \| g_k \|^2 . \end{aligned}$$

Dividing by $\left(g_k^T d_k \right)^2$ in the both sides of this equality, then from (6), (7), we obtain

$$\begin{aligned} \frac{\|d_k\|^2}{\|g_k\|^4} &= \frac{\left(\beta_k \right)^2 \|d_{k-1}\|^2 - 2\theta_k d_k^T g_k - \theta_k^2 \|g_k\|^2}{\|g_k\|^4} \\ &\leq \frac{\|d_{k-1}\|^2}{\|g_{k-1}\|^4} - \frac{\left(\theta_k - 1 \right)^2}{\|g_k\|^2} + \frac{1}{\|g_k\|^2} \end{aligned}$$

$$\le \frac{\|d_{k-1}\|^2}{\|g_{k-1}\|^4} + \frac{1}{\|g_k\|^2}$$
$$\le \sum_{i=0}^{k-1} \frac{1}{\|g_i\|^2}$$
$$\le \frac{k}{\varepsilon^2}$$

The last inequalities implies

$$\sum_{k\ge 1} \frac{\|g_k\|^4}{\|d_k\|^2} \ge \varepsilon^2 \sum_{k\ge 1} \frac{1}{k} = +\infty$$

which contradicts the result of Lemma 1. Therefore,

$$\lim_{k\to\infty} \inf \|g_k\| = 0$$

The proof of the desired result is completed. ■

4 Remarks on the Existent Methods

In this section, we shall give some remarks on the existent spectral conjugate gradient methods. It is shown that they are special cases of the proposed method in this paper.

It is first noted that, in [7], the conjugate and spectral parameters of the search direction are taken, respectively, as follows:

$$\beta_k = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}, \qquad \theta_k = \frac{d_{k-1}^T y_{k-1}}{\|g_{k-1}\|^2}$$

The step size α_k in [7] is chosen by

$$\alpha_k = -\frac{\delta g_k^T d_k}{\|d_k\|_{Q_k}^2} \tag{14}$$

where $\|d_k\|_{Q_k} = \sqrt{d_k^T Q_k d_k}$, $\delta \in \left(0, \frac{v_{\min}}{L}\right)$ and $\frac{\delta L}{v_{\min}} < 1$, L is a Lipschitz constant, $\{Q_k\}$ is a sequence of positive definite matrices satisfying $v_{\min} d_k^T d_k \le d_k^T Q_k d_k \le v_{\max} d_k^T d_k$, and $v_{\min}$ 、 $v_{\max}$ are positive constants.

From Lemma 1 in [7], we have

$$d_k^T g_k = -\|g_k\|^2$$

From (14) and Lemma 1 of [7], it follows that

$$\alpha_k = -\frac{\delta g_k^T d_k}{\|d_k\|_{Q_k}^2} \le \frac{\delta \|g_k\|^2}{v_{\min}\|d_k\|^2}$$

$$\tilde{\alpha}_k > \mu \frac{\|g_k\|^2}{\|d_k\|^2}$$

and

$$0 < c_k = \frac{\alpha_k}{\tilde{\alpha}_k} \le \frac{\delta}{\mu v_{\min}} < \frac{1}{\mu L}$$

Therefore, the sequence $\{c_k\}$ is bounded.

On the other hand, it is obtained that

$$d_k^T g_k = -\|g_k\|^2$$

$$\beta_k = \frac{\|g_k\|^2}{\|g_{k-1}\|^2} \le \frac{\|g_k\|^2}{\|g_{k-1}\|^2}$$

and

$$\alpha_k = c_k \tilde{\alpha}_k$$

where $c_k < \dfrac{1}{\mu L}$ is bounded. In other words, Assumption 2 holds.

From the above discussion, it is seen that the convergence result in [7] is a special case of that obtained in this paper.

Secondly, we discuss the modified method A in [6]. The search direction of the modified method A in [6] is

$$d_k = \begin{cases} -g_0, & if \quad k = 0, \\ -\theta_k g_k + \beta_k d_{k-1}, & if \quad k \ge 1, \end{cases}$$

where

$$\theta_k = \frac{(g_k - g_{k-1})^T d_{k-1}}{\|g_{k-1}\|^2},$$

and

$$\beta_k = \frac{\|g_k\|^2}{\|g_{k-1}\|^2}.$$

We can prove the following result.

Lemma 2: Suppose that d_k is determined by the modified method A in [6]. Then, the following result

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

holds for any $k \geq 0$.

Proof: Firstly, for $k = 0$, it is easy to see that is true since $d_0 = - g_0$.

Secondly, assume that

$$g_{k-1}{}^T d_{k-1} = - \|g_{k-1}\|^2, \forall \ k \geq 1$$

holds for $k - 1$. Then, from the modified method A of in [6], it follows that

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

Thus, it is also true with $k - 1$ replaced by k. By mathematical induction method, we obtain the desired result.

In the other hand, in [6], the step size

$$a_k = - \frac{- g_k^T d_k}{2L\|d_k\|^2}$$

where L is a Lipschitz constant, so

$$0 < c_k = \frac{a_k}{\tilde{a}_k} < \frac{1}{2mL} = \frac{1}{2r\,(1 - d_1)}$$

Therefore, it is obtained that

$$d_k^T g_k = - \|g_k\|^2 .$$

$$b_k = \frac{\|g_k\|^2}{\|g_{k-1}\|^2} \leq \frac{\|g_k\|^2}{\|g_{k-1}\|^2} .$$

and

$$a_k = c_k \partial/\rho_k$$

where $c_k < \dfrac{1}{2r\left(1 - s_1\right)}$ is bounded. That is Assumption 2 holds.

From the above discussion, it is clear that the convergence result in the modified method A in [6] is a special case of that obtained in this paper.

We now in a position to review the method presented in [14]. In [14], the step size a_k is chosen to be the largest component in the set $\left\{r^j, j = 0,1,...\right\}$ such that

$$f(x^k + a_k d_k) \le f(x_k) + d_1 a_k g_k^T d_k - d_2 a_k^2 \| d_k \|^2 . \tag{15}$$

We first prove the following theorem, which shows that the line search rule (15) is actually the standard Armijo line search (9).

Theorem 2: Let a_k be the largest component in the set $\left\{r^j, j = 0,1,...\right\}$ such that

$$f(x_k + a_k d_k) \le f(x_k) + d_1 a_k g_k^T d_k - d_2 a_k^2 \| d_k \|^2$$

Then, there a constant scalar $s \in \left(0,1\right)$ such that a_k satisfies

$$f(x_k + a_k d_k) \le f(x_k) + s\, a_k g_k^T d_k . \tag{16}$$

Proof: Firstly, from (2.3) in [15], it follows that for all $k > 0$,

$$d_k^T g_k = -\| g_k \|^2$$

Combined with the result of Lemma 3.1 in [14], which says $a_k \ge c \dfrac{\| g_k \|^2}{\| d_k \|^2}$, where

$c = \min\left\{1, \dfrac{(1 - d_1) r}{L + d_2}\right\}$, $d_1, d_2 > 0, r \in (0,1)$, we have

$$\begin{aligned} f(x_k + a_k d_k) &\le f(x_k) + d_1 a_k g_k^T d_k - d_2 a_k^2 \| d_k \|^2 \\ &\le f(x_k) + d_1 a_k g_k^T d_k - d_2 a_k c \| g_k \|^2 \\ &= f(x_k) + d_1 a_k g_k^T d_k + d_2 a_k c g_k^T d_k \\ &= f(x_k) + (d_1 + d_2 c) a_k g_k^T d_k \end{aligned} \tag{17}$$

Next, we prove that $d_1 + d_2 c$ is a constant in the interval $\left(0,1\right)$.

On one hand,

$$\begin{aligned}\delta_1+\delta_2\chi &= \min\left\{\delta_1+\delta_2, \delta_1+\frac{1-\delta_1}{L+\delta_2}\delta_2\rho\right\}\\ &= \min\left\{\delta_1+\delta_2, \delta_1+\frac{\delta_2\rho}{L+\delta_2}(1-\delta_1)\right\}\end{aligned}$$

On the other hand, since $\frac{\delta_2}{L+\delta_2}<1$, and $\delta_1+\frac{\delta_2\rho}{L+\delta_2}(1-\delta_1)=\delta_1\cdot 1+(1-\delta_1)\cdot\frac{\delta_2\rho}{L+\delta_2}$ is a convex combination of 1 and $\frac{\delta_2}{L+\delta_2}$, it is clear that $0<\delta_1+\delta_2\chi<1$.

Therefore, there exists a constant scalar $\sigma=\delta_1+\delta_2\chi\in(0,1)$ such that α_k satisfies

$$f(x_k+\alpha_k d_k)\le f(x_k)+\sigma\alpha_k g_k^T d_k$$

Remark 3: *Theorem 2 indicates that the line search proposed in* [14] *is not a modification of the standard Armijo line search. Thus, it is concluded that the efficiency of the developed algorithm in* [14] *does not result from the used line search rule.*

In addition, it is noted that, in [14], the conjugate parameter is chosen as $\beta_k=\frac{\|g_k\|^2}{\|g_{k-1}\|^2}$.Whence, it is easy to prove that

$$\begin{aligned}&d_k^T g_k=-\|g_k\|^2.\\ &\beta_k=\frac{\|g_k\|^2}{\|g_{k-1}\|^2}\le\frac{\|g_k\|^2}{\|g_{k-1}\|^2}\\ &\alpha_k=c_k\tilde{\alpha}_k\end{aligned}$$

where $c_k=1$ is bounded. Therefore, Assumption 2 is satisfied, which implies that the convergence result in [14] also is a special case of that obtained in this paper.

Remark 4: *From the above discussion on the existent three algorithms, our algorithm is an extension of them even if for the simplest case (3). Different from the other similar spectral conjugate gradient methods available in the literature, the values of the spectral and conjugacy parameters in the extended method (3) can be chosen in a suitable range, instead of fixed expression for each parameter.*

5 Final Remarks

In this paper, we have proposed an extended spectral conjugate gradient method. It has been shown that the other three classes of existent methods are the special cases of the presented method. Some suitable conditions were presented to ensure the global convergence of the developed method.

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Competing Interests

Authors have declared that no competing interests exist.

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