A New Nonlinear Conjugate Gradient Coefficient for Unconstrained Optimization

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Abstract

In this paper, we suggest a new nonlinear conjugate gradient method for solving large scale unconstrained optimization problems. We prove that the new conjugate gradient coefficient $\beta_k$ with exact line search is globally convergent. Preliminary numerical results with a set of 116 unconstrained optimization problems show that $\beta_k$ is very promising and efficient when compared to the other conjugate gradient coefficients Fletcher - Reeves ($FR$) and Polak -Ribiere – Polyak (PRP).

Keywords: Conjugate gradient coefficient, exact line search, global convergence, large scale, unconstrained optimization

1. Introduction

In this paper, we focus our attention on the unconstrained optimization problem,

$$\min_{x \in \mathbb{R}^n} f(x)$$

(1.1)

where $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable function and $\mathbb{R}^n$ denotes an $n$-dimensional Euclidean space. We denote by $g(x)$, the gradient of $f$ at $x$. The
conjugate gradient (CG) method is the best methods for solving (1.1), especially when the dimension is large. The iterates of the CG method for solving (1.1) are obtained by

\[ x_{k+1} = x_k + \alpha_k d_k, \quad k = 0, 1, 2, \ldots \]

Where \( x_k \) is current iterate point and the \( \alpha_k \) is step size. The step size is computed by carrying out some line search, for example, the exact line search where,

\[ \alpha_k = \arg \min_{\alpha > 0} f(x_k + \alpha d_k) \]

The \( d_k \) is the search direction defined by

\[ d_k = \begin{cases} 
  -g_k & \text{if } k = 0, \\
  -g_k + \beta_k d_{k-1} & \text{if } k \geq 1,
\end{cases} \]

Where \( g_k = g(x_k) \) and \( \beta_k \) is a scalar. The most well-known classical formula for \( \beta_k \) are the Hestenes-Stiefel (HS) method [11], the Fletcher-Reeves (FR) method [7], the Polak-Ribiere-Polyak (PRP) method [15, 16], the conjugate descent (CD) method[6], the Liu–Storey (LS) method [14] and the Dai–Yuan (DY) method [2]. The parameters of these \( \beta_k \) as follows

\[ \beta^{HS}_k = \frac{g_k^T (g_k - g_{k-1})}{(g_k - g_{k-1})^T d_{k-1}} \]

\[ \beta^{FR}_k = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} \]

\[ \beta^{PRP}_k = \frac{g_k^T (g_k - g_{k-1})}{g_{k-1}^T g_{k-1}} \]

\[ \beta^{CD}_k = \frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \]

\[ \beta^{LS}_k = \frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T g_{k-1}} \]

\[ \beta^{DY}_k = \frac{g_k^T g_k}{(g_k - g_{k-1})^T d_{k-1}} \]

The most studied properties of CG methods are its global convergence properties. Zoutendijk [22] and Powell [17] proved that FR method with exact line search is globally convergent. Zhang et al [13], Proposed a modified FR method \( MFR \) which
A new nonlinear conjugate gradient coefficient is globally convergent under inexact line search. Polyak [16] and Powell [18] showed that PRP has a good numerical performance, but does not have such good convergence property. Touati-Ahmed and Storey [20], Gilbert and Nocedal [8] gave another way to discuss the global convergence of the PRP method with the weak Wolfe – Powell line search, where the parameter $\beta_k$ in (1.6) is not allowed to be negative, $\beta_k = \max\{\beta_k^{PRP}, 0\}$, therefore, during the past few years, many authors have been investigated to create new formulas for $\beta_k$ [3, 4, 9, 10, 19, 21].

In this paper, we will show a new $\beta_k$ in section 2. In section 3, we will study the sufficient descent condition and the global convergence proof of the new $\beta_k$. In section 4, we present the numerical results and discussion. Finally, we present the conclusions in section 5.

2. New $\beta_k$ parameter and algorithm

In this section, we present a modified PRP method which is known as $\beta_k^{MRM}$, where $MRM$ denotes Mohamed, Rivaie and Mustafa, $\beta_k^{MRM}$ is defined by,

$$\beta_k^{MRM} = \frac{g_k^T (g_k - \|g_k\| g_{k-1})}{\|g_{k-1}\|^2 + \|g_k^T d_{k-1}\|^2}$$

(2.1)

The following algorithm is a general algorithm for solving optimization by CG methods.

Algorithm (2.1)

Step 1: Given $x_0 \in \mathbb{R}^n, \epsilon \geq 0$, set $d_0 = -g_0$ if $\|g_0\| \leq \epsilon$ then stop.

Step 2: Compute $\alpha_k$ by exact line search (1.3).

Step 3: Let $x_{k+1} = x_k + \alpha_k d_k$, $g_{k+1} = g(x_{k+1})$ if $\|g_{k+1}\| < \epsilon$ then stop.

Step 4: Compute $\beta_k$ by formula (2.1), and generate $d_{k+1}$ by (1.4).

Step 5: Set $k = k + 1$ go to Step 2.

The following assumptions are often used in the studies of the conjugate gradient methods.

Assumption A. $f(x)$ is bounded from below on the level set $\Omega = \{x \in \mathbb{R}^n, f(x) \leq f(x_0)\}$, where $x_0$ is the starting point.

Assumption B. In some neighbourhood $N$ of, the objective function is continuously differentiable, and its gradient is Lipschitz continuous, that is there exists a constant $L > 0$ such that

$$\|g(x) - g(y)\| \leq L\|x - y\| \forall x, y \in N.$$  

(2.2)
3. The Global Convergence properties

In this section, we study the global convergent properties of $\beta_k^{MRM}$, first we need to simplify the $\beta_k^{MRM}$, so that the proof will be easier. From (2.1) we know that

$$\beta_k^{MRM} = \frac{g_k^T (g_k - \frac{1}{\|g_{k-1}\|} g_{k-1})}{\|g_{k-1}\|^2 + g_k^T d_{k-1}}$$

Thus we get, $\beta_k^{MRM} \geq 0$

Also

$$\beta_k^{MRM} = \frac{\|g_k\|^2 - \|g_{k-1}\|^2 \|g_k g_{k-1}\|}{\|g_{k-1}\|^2 + g_k^T d_{k-1}} \geq \frac{\|g_k\|^2 - \|g_{k-1}\|^2 \|g_k\| \|g_{k-1}\|}{\|g_{k-1}\|^2 + g_k^T d_{k-1}} = 0$$

Hence we obtain

$$0 \leq \beta_k^{MRM} \leq \frac{2\|g_k\|^2}{\|g_{k-1}\|^2}$$

The following lemmas are very useful in the process of the studies on the conjugate gradient methods

**Lemma 3.1.**
Suppose that Assumptions A and B hold, let $x_k$ be generated by Algorithm 2.1 where, $d_k$ satisfies $g_k^T d_k < 0$ for all $k$, and $\alpha_k$ is obtained by (1.3), then,

$$\sum_{k=0}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty$$

This theorem show that $B_k^{MRM}$ has an advancement that the directions will approach to the steepest descent directions while the step length $\alpha_k$ is small.

**Theorem 3.1.**
Suppose that Assumptions A and B hold, $\{x_k\}$ generated by the Algorithm 2.1, where the step size $\alpha_k$ is determined by the exact line search (1.3). Then (3.1) holds for all $k \geq 0$. 
Proof. Suppose that for all \( k \), \( g_k \neq 0 \). If \( k = 0 \) then \( g_0^T d_0 = g_0^T (-g_0) = -\|g_0\|^2 \). If at a point \( x_k \), \( d_k \) is not a descent direction, then by the exact line search, we have \( x_{k+1} = x_k \) which implies \( g_{k+1} = g_k \). From (2.1), we have \( b_k^{\text{MRM}} = 0 \). This means that at those points the directions will turn out to be the steepest descent directions. Those points are denoted by \( P_1 = \{ x_k : b_k^{\text{MRM}} = 0 \} \) and the other points are denoted by \( P_2 = \{ x_k : b_k^{\text{MRM}} \neq 0 \} \).

For all the points in \( P_1 \), since the directions are the steepest descent directions, from Lemma 2.1, we have

\[
\sum_{x_i \in P_1} (g_i^T d_i)^2 < \infty
\]  

(3.2)

The same as the above proof, for the points in \( P_2 \), we also have

\[
\sum_{x_i \in P_2} (g_i^T d_i)^2 < \infty
\]  

(3.3)

From (3.2) and (3.3) we have,

\[
\sum_{k=0}^n (g_k^T d_k)^2 = \sum_{x_i \in P_1} (g_i^T d_i)^2 + \sum_{x_i \in P_2} (g_i^T d_i)^2 < \infty
\]

The proof is completed.

Theorem 3.2

Suppose that Assumptions A and B hold, the sequence \( \{ x_k \} \) is generated by Algorithm 2.1, if \( \| x_k \| = \| x_k d_k \| \to 0 \) while \( k \to \infty \), then

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

(3.4)

Proof. Let \( \theta_k \) be the angle between \( -g_k \) and \( d_k \), where

\[
\cos \theta_k = \frac{-g_k^T d_k}{\| g_k \| \| d_k \|}
\]

then by the exact line search, we have \( g_k^T d_{k-1} = 0 \), where the search direction defined by (1.4), the following relations hold true:

\[
\| d_k \| = \sec \theta_k \| g_k \|, \quad \beta_{k+1} \| d_k \| = \tan \theta_{k+1} \| g_{k+1} \|
\]

So we have

\[
\tan \theta_{k+1} = \beta_{k+1} \sec \theta_k \| g_{k+1} \| \quad \| g_{k+1} \| \quad g_{k+1} = \frac{g_k^T (g_{k+1} - \| g_{k+1} \| g_k)}{\| g_{k+1} \| \| g_k \|}
\]

\[
\tan \theta_{k+1} \leq \sec \theta_k \| g_{k+1} \| \| g_{k+1} \| \| g_k \| = \sec \theta_k \| g_{k+1} \| \| g_k \|
\]

(3.5)
If (3.4) does not hold, then, for all \( k \), there exists \( c > 0 \) such that
\[
\|g_k\| \geq c
\]  
(3.6)

By \( \|s_k\| \rightarrow 0 \) and Lipschitz condition (2.2), there must exist an integer \( M \geq 0 \) for all \( k \geq M \), such that
\[
\|g_{k+1} - g_k\| \geq \frac{1}{4} c
\]  
(3.7)

Combining (3.5) and (3.7), we obtain
\[
\tan \theta_{k+1} \leq \frac{1}{2} \sec \theta_k
\]  
(3.8)

We know that, for all \( \theta \in [0, \frac{\pi}{2}) \), the following inequality holds:
\[
\sec \theta \leq 1 + \tan \theta
\]  
(3.9)

From (3.8) and (3.9) we get,
\[
\tan \theta_{k+1} \leq \frac{1}{2} (1 + \tan \theta_k)
\]  
(3.10)

Utilizing (3.10) induces,
\[
\tan \theta_{k+1} \leq \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \ldots + \left( \frac{1}{2} \right)^{k+1-m} + \left( \frac{1}{2} \right)^{k+1-m} \tan \theta_m \leq 1 + \tan \theta_m
\]

From this result, we note that the angle \( \theta_k \) must be always less than some angle \( \theta \) where, \( \theta < \frac{\pi}{2} \), but by the Theorem 3.1, we have
\[
\sum_{k=0}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} = \sum_{k=0}^{\infty} \|g_k\|^2 (\cos \theta_k)^2 < \infty
\]

This implies \( \lim \inf_{k \to \infty} \|g_k\| = 0 \), which contradicts (3.6). The proof is completed.

4. Numerical results and discussions

In this section, we present the computational performance of a MATLAB program on a set of 116 unconstrained optimization test problems. We selected 24 test functions considered in Andrei [1], each of them is tested in different variables. We performed a comparison with two CG methods Fletcher – Reeves (FR) and Polak-Ribiere-Polyak (PRP), we considered \( \varepsilon = 10^{-6} \) and the gradient value as the stopping criteria as Hillstrom [12] suggested that \( \|g_k\| \leq \varepsilon \) as the stopping criteria. For each of the test functions problem, we used four initial points, starting from a closer point to the solution and moving on to the one that is furthest from it. A list of problem functions and the initial points used are shown
in table 1, where the exact line search was used to compute the step size. The CPU processor used was Intel (R) Core™ i3-M350 (2.27GHz), with RAM 4 GB. In some cases, the computation stopped due to the failure of the line search to find the positive step size, and thus it was considered a failure. Numerical results are compared relative on the CPU time and number of iteration. The performance results are shown in Figs. 1 and 2 respectively, using a performance profile introduced by Dolan and More [5].

| No | Function     | Dimension | Initial points               |
|----|--------------|-----------|------------------------------|
| 1  | Three Hump   | 2         | (-10,-10),(10,10),(20,20),(40,40) |
| 2  | Six Hump     | 2         | (-10,-10),(-8,8),(8,8),(10,10)  |
| 3  | Booth        | 2         | (10,10),(25,25),(50,50),(100,100) |
| 4  | Treccani     | 2         | (5,5),(10,10),(20,20),(50,50)  |
| 5  | Zettl        | 2         | (5,5),(10,10),(20,20),(50,50)  |
| 6  | Diagonal 4   | 2, 4, 10,100,500,1000 | (1,...,1),(3,...,3),(6,...,6),(12,...,12) |
| 7  | Perturbed Qua.| 2, 4, 10,100,500,1000 | (1,...,1),(3,...,3),(5,...,5),(10,...,10) |
| 8  | E-Himmelblau | 10,100,500,1000,10000 | (50,...,50),(70,...,70),(100,...,100),(125,...,125) |
| 9  | E-Rosenbrock | 10,100,500,1000,10000 | (13,...,13),(25,...,25),(30,...,30),(50,...,50) |
| 10 | Shallow      | 10,100,500,1000,10000 | (10,...,10),(25,...,25),(50,...,50),(70,...,70) |
| 11 | E-Tridiagonal| 10,100,500,1000,10000 | (6,...,6),(12,...,12),(17,...,17),(20,...,20) |
| 12 | G-Tridiagonal| 2,4,10,100 | (7,...,7),(10,...,10),(13,...,13),(21,...,21) |
| 13 | E-white-Holst| 2,4,10,100,500,1000,10000 | (3,...,3),(5,...,5),(7,...,7),(10,...,10) |
| 14 | G-Quartic    | 2,4,10,100,500,1000,10000 | (1,...,1),(2,...,2),(5,...,5),(7,...,7) |
| 15 | E-Powell     | 4,20,100,500,1000 | (2,...,2),(4,...,4),(6,...,6),(8,...,8) |
| 16 | E-Denschnb   | 2,4,10,100,500,1000,10000 | (8,...,8),(13,...,13),(30,...,30),(50,...,50) |
| 17 | Hager        | 2,4,10,100 | (7,...,7),(10,...,10),(15,...,15),(23,...,23) |
| 18 | E-Penalty    | 2,4,10,100 | (80,...,80),(10,...,100),(111,...,111),(150,...,150) |
| 19 | Quadric QF2  | 2,4,10,100,500,1000 | (5,...,5),(20,...,20),(50,...,50),(100,...,100) |
| 20 | E-QP2        | 2,4,10,100,500,1000 | (10,...,10),(20,...,20),(30,...,30),(50,...,50) |
| 21 | E-Beale      | 2,4,10,100,500,1000,10000 | (-1,...,-1),(3,...,3),(7,...,7),(10,...,10) |
| 22 | Diagonal 2   | 2,4,10,100,500,1000 | (1,...,1),(5,...,5),(10,...,10),(15,...,15) |
| 23 | Raydan1      | 2,4,10,100 | (1,...,1),(3,...,3),(7,...,7),(10,...,10) |
| 24 | Sum Squares  | 2,4,10,100,500,1000 | (1,...,1),(3,...,3),(7,...,7),(10,...,10) |

According to the rules considered in [5], we know that the method whose performance profile plot on top right will be better than the rest of the other methods. Figures 1-2 show that the performances of these methods are relative to the number of iteration and the CPU time. From figures 1-2, it is easy to see that MRM is the best among the two methods FR and PRP, the performance of PRP seems to be faster than MRM, but it can solve only 93% of the problems and FR solved only 70%, where MRM can solve all the test problems and reach 100%, the performance of MRM lies between FR and PRP. In other words, MRM method is competitive to the other two methods and its notable formula.
5. Conclusion and further research

This paper gives a new conjugate gradient method for solving unconstrained optimization problems. Under the exact line search, this $\beta_k$ possesses the global convergence condition. Numerical results show that our method is competitive to other two conjugate gradient methods, Fletcher Reeves (FR) and Polak Ribiere Polyak (PRP), and come out with best numerical results.

For further research, we should study the new method with the strong Wolfe-Powell line search.

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