A NEW NONLINEAR CONJUGATE GRADIENT METHOD WITH EXACT LINE SEARCH FOR UNCONSTRAINED OPTIMIZATION

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ABSTRACT

This paper deals with a new nonlinear conjugate gradient method for solving large-scale unconstrained optimization problems. We prove that the new conjugate gradient coefficients β_k with exact line search is globally convergent. Preliminary numerical results show that β_k is very efficient when compared to the other classical conjugate gradient coefficients *FR*,*PRP*, *NPRP*, and *RMIL*.

Keywords: Exact line search, Conjugate gradient coefficient, Global convergence.

1. INTRODUCTION

Consider the following n-variables unconstrained optimization problem:

$$\min\left\{f(x) : x \in R^n\right\}, \tag{1}$$

where R^n denotes an n-dimensional Euclidean space and $f : R^n \to R$ is smooth,and its gradient $g(x)$ is available. The conjugate gradient (CG) method is a powerful method for solving (1), because of its simplicity and low memory requirement, especially when the dimension is large. The iterative formula of the conjugate gradient methods for solving (1) is given by

$$x_{k+1} = x_k + \alpha_k d_k, \qquad k = 0,1,2,... \tag{2}$$

where x_k is current iterate point and α_k is a step length which is computed by carrying out a line search, for example, the exact line search where,

$$\alpha_k = arg \min_{\alpha \geq 0} f(x_k + \alpha d_k) \tag{3}$$

The d_k is the search direction defined by

$$d_k = \begin{cases} -g_k & \text{if} \quad k = 0, \\ -g_k + \beta_k d_{k-1} & \text{if} \quad k \geq 1, \end{cases} \tag{4}$$

where $g_k = g(x_k)$ and β_k is a parameter that determines the different conjugate gradient methods, for example, well-known cases of β_k can be taken as:

$$\beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{(g_k - g_{k-1})^T d_{k-1}} \quad \text{(Hastens - Stiefel[1], 1952)} \tag{5}$$

$$\beta_k^{FR} = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} \quad \text{(Fletcher-Reeves[2], 1964)} \tag{6}$$

$$\beta_k^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{g_{k-1}^T g_{k-1}} \quad \text{(PolakRibierePolyak[3, 4], 1969)} \tag{7}$$

$$\beta_k^{CD} = -\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \quad \text{(Conjugate Descent[5],1987)} \tag{8}$$

$$\beta_k^{LS} = -\frac{g_k^T (g_k - g_{k-1})}{d_{k-1}^T g_{k-1}} \quad \text{(Liu – Storey[6], 1991)} \tag{9}$$

$$\beta_k^{DY} = \frac{g_k^T g_k}{(g_k - g_{k-1})^T d_{k-1}} \quad \text{(Dai – Yuan [7], 1999)} \tag{10}$$

The convergence behaviour of the above formulas with some line search conditions has been studied by many authors for many years (see [8-14]).Zoutendijk[15] and Powell [16] proved that FR method with exact line search is globally convergent. Polak and Ribie`re[3] proved that the PRP method with the exact line search is globally convergent. But Powell [4] showed that there exist non-convex functions on which the PRP method does not converge globally. He suggested that β_k should not be less than zero. Gilbert and Nocedal[17] proved that the modified PRP method $\beta_k = \max\{\beta_k^{PRP}, 0\}$ is globally convergent with the Wolfe–Powell line search. There are many new formulas that have been studied by many authors (see [18-28] etc.)

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

2.NEW β_k PARAMETER AND ALGORITHM

Recently, Wei et al. [25]have presented a variant of the *PRP* method which is called the *WYL* method. Zhang [29] based on *WYL*has improved a new conjugate gradient method called,*NPRP* and he proved that the *NPRP* method satisfies descent condition under strong Wolfe line search. Zhang et al. [14] proposed another modified method known as *MPRP* ,and Dai and Wen [20] propose modified *NPRP* method known as *DPRP*. Rivaieet al.[30] proposed another modified method known as *RMIL*. In this paper, enlightened by the above ideas, a Modified *PRP* Conjugate Gradient Method will be proposed as follows:

$$\beta_k^{HRM} = \frac{g_k^T \left(g_k - \dfrac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{u\|g_{k-1}\|^2 + (1-u)\, \|d_{k-1}\|^2} \qquad , u = 0.4 \qquad (11)$$

where, *HRM* denotes the authorsHamoda, Rivaie and Mustafa.

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

Algorithm 2.1

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

Step 2: Compute α_k by exact line search (3).

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

Step 4: Compute β_k by formula (11) ,and generate d_{k+1} by (4).

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

3. GLOBAL CONVERGENCE ANALYSIS

In this section, we study the global convergent properties of β_k and begin with the sufficient descent condition.

3.1 Sufficient descent condition

For the sufficient descent condition to hold,

$$g_k^T d_k \le -c\|g_k\|^2 \ \ \forall k \ge 0, c > 0 \tag{12}$$

The following theorem shows that our new formula with exact line search possess the sufficient descent condition.

Theorem 3.1. Let $\{x_k\}$ and $\{d_k\}$ be sequence generated by algorithm 2.1, then (12) holds for all $k \ge 0$.

Proof

We proof by induction, that if $k = 0$ then $g_0^T d_0 = -c\|g_0\|^2$

Hence, the condition holds true; now we need to prove that:

$$g_k^T d_k \le -c\|g_k\|^2 \ \ \text{for } k \ge 1$$

From (4) we have $d_{k+1} = -g_{k+1} + \beta_{k+1} d_k$

Multiply both sides by g_{k+1}^T

$$g_{k+1}^T d_{k+1} = g_{k+1}^T(-g_{k+1} + \beta_{k+1} d_k) = -\|g_{k+1}\|^2 + \beta_{k+1} g_{k+1}^T d_k \tag{13}$$

For exact line search, we know that $g_{k+1}^T d_k = 0$. Thus $g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2$

Hence this condition holds true for $k+1$. Therefore, the sufficient descent condition holds. □

3-2 Global convergence properties

To study global convergence properties, we need to simplify the β_k^{HRM}, so that the proof will be easier. From (11) we know that

$$\beta_k^{HRM} = \frac{g_k^T \left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{u\|g_{k-1}\|^2 + (1-u)\ \|d_{k-1}\|^2} \qquad ,u = 0.4 \tag{14}$$

Using triangle inequality and Cauchy-Schwarz inequality, to get

$$\beta_k^{HRM} = \frac{g_k^T \left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2} \geq \frac{\|g_k\|^2 - \frac{\|g_k\|}{\|g_{k-1}\|}\left|g_k^T g_{k-1}\right|}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2}$$

$$\geq \frac{\|g_k\|^2 - \frac{\|g_k\|}{\|g_{k-1}\|}\|g_k\|\|g_{k-1}\|}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2} = 0 \tag{15}$$

Thus we get

$$\beta_k^{HRM} \geq 0$$

Also from (14) using triangle inequality and Cauchy-Schwarz inequality, to get

$$\beta_k^{HRM} = \frac{g_k^T \left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} g_{k-1}\right)}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2} \le \frac{\|g_k\|^2 + \frac{\|g_k\|}{\|g_{k-1}\|}\left|g_k^T g_{k-1}\right|}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2}$$

$$\le \frac{\|g_k\|^2 + \frac{\|g_k\|}{\|g_{k-1}\|}\|g_k\|\|g_{k-1}\|}{u\|g_{k-1}\|^2 + (1-u)\|d_{k-1}\|^2} \le \frac{2\|g_k\|^2}{u\|g_{k-1}\|^2}$$

Hence we obtain

$$0 \le \beta_k^{HRM} \le \frac{5\|g_k\|^2}{\|g_{k-1}\|^2} \tag{16}$$

To prove the global convergence of the CG method, we first make the following assumption.

Assumption 3.1

(i) The level set $\Omega = \{x \in R^n, f(x) \le f(x_0)\}$ is bounded, where x_0 is the starting point.

(ii) In some neighbourhood of Ω, the objective function is continuously differentiable, and its gradient is Lipschitz continuous, that is there exists a constant $L > 0$ such that

$$\|g(x) - g(y)\| \le L\|x - y\| \ \forall x, y \in N \tag{17}$$

The following lemma which is famous for global convergence properties is by Zoutendijk[15].

Lemma 3.1

Suppose Assumption (3.1) holds, let x_k be generated by Algorithm (2.1) and d_k satisfy $g_k^T d_k < 0$ for all k, and α_k is obtained by (3), then we have

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

Theorem 3.2. Suppose that Assumptions (3.1) holds, the sequence $\{x_k\}$ is generated by Algorithm 2.1, if $\|S_k\| = \|\alpha_k d_k\| \to 0$ while $k \to \infty$, then

$$\lim_{k\to\infty} \inf \|g_k\| = 0 \tag{18}$$

Proof

Let θ_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 (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

$$\tan\theta_{k+1} = \beta_{k+1}^{HRM} \sec\theta_k \frac{\|g_k\|}{\|g_{k+1}\|} = \sec\theta_k \frac{\|g_k\|}{\|g_{k+1}\|} \frac{g_{k+1}^T(g_{k+1} - \frac{\|g_{k+1}\|}{\|g_k\|} g_k)}{u\|g_k\|^2 + (1-u)\|d_k\|^2}$$

$$\leq \sec\theta_k \frac{\|g_{k+1}\|\|g_k\|\left\|g_{k+1} - \frac{\|g_{k+1}\|}{\|g_k\|} g_k\right\|}{u\|g_{k+1}\|\|g_k\|^2}$$

$$= \sec\theta_k \frac{\left\|g_{k+1} - g_k + g_k - \frac{\|g_{k+1}\|}{\|g_k\|} g_k\right\|}{u\|g_k\|} \leq \sec\theta_k \frac{\|g_{k+1} - g_k\| + \left|\,\|g_k\| - \|g_{k+1}\|\,\right|}{u\|g_k\|}$$

$$\tan\theta_{k+1} \leq \sec\theta_k \frac{5\|g_{k+1} - g_k\|}{\|g_k\|} \tag{19}$$

If (18) does not hold, then, for all k, there exists $c > 0$ such that

$$\|g_k\| \geq c \tag{20}$$

By $\|S_k\| \to 0$ and Lipschitz condition (17), there must exist an integer $M \geq 0$ for all $k \geq M$, such that

$$\|g_{k+1} - g_k\| \leq \frac{1}{10} c \tag{21}$$

Combining (19) and (21), we obtain

$$\tan\theta_{k+1} \leq \frac{1}{2} \sec\theta_k \tag{22}$$

We know that, for all $\theta \in [0, \frac{\pi}{2})$, the following inequality holds:

$$\sec\theta \le 1 + \tan\theta \tag{23}$$

from (22) and (23) we get,

$$\tan\theta_{k+1} \le \frac{1}{2}(1 + \tan\theta_k) \tag{24}$$

Utilizing (24) induce,

$$\tan\theta_{k+1} \le \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + ... + \left(\frac{1}{2}\right)^{k+1-m} + \left(\frac{1}{2}\right)^{k+1-m} \tan\theta_m \le 1 + \tan\theta_m$$

From this result, we note that the angle θ_k must always be less than some angle θ where, $\theta < \frac{\pi}{2}$, but by the Lemma (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 that, $\lim_{k\to\infty} \inf \|g_k\| = 0$, which contradicts (20). The proof is completed. Therefore, the new formula *HRM* with the exact line search is globally convergent. Also in [31] the global convergence of *HRM* with strong Wolfe-Powell line search was proved.

4. NUMERICAL RESULTS AND DISCUSSIONS

In this section, we used 32th test functions considered in [32-34] to find the computational results to analyze the efficiency of HRM. We performed a comparison with four CG methods*FR, PRP, RMIL,*and*NPRP*.We considered $\varepsilon = 10^{-6}$ and the gradient value as the stopping criteria as Hillstrom[35] suggested that $\|g_k\| \le \varepsilon$ as the stopping criteria. For each of the test functions, 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 functions and the initial points used are shown in table 1, where all the problems are solved by MATLAB program. We used the exact line search to compute the step size. The CPU processor used was Intel (R) CoreTM 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 iterations. The performance results are shown in figure1 and figure 2 respectively, using a performance profile introduced by Dolan and More [36].

TABLE 1. A LIST OF PROBLEM FUNCTIONS

No	**Function**	**Dimension**	**Initial points**
1	Three Hump	2	-10,10,20,40
2	Six Hump	2	-10,10, -8, 8
3	Booth	2	10,25,50,100
4	Treccani	2	5, 10, 20, 50
5	Zettl	2	5, 10, 20, 50
6	Diagonal 4	2,4, 10,100,500,1000	1, 3, 6,12

7	Perturbed Quadratic	2,4, 10,100,500,1000	1,3,5, 10
8	Extended Himmelblau	10,100,500,1000,10000	50,70,100, 125
9	Extended Rosenbrock	2,4, 10,100,500,1000,10000	13,25,30,50
10	Shallow	2,4, 10,100,500,1000,10000	10,25,50, 70
11	Extended Tridiagonal1	2,4, 10,100,500,1000,10000	6,12,17,20
12	Generlyzed Tridiagonal1	2,4,10,100	7,10, 13,21
13	Extended white & Holst	2,4,10,100,500,1000,10000	3,5,7,10
14	Generalized Quartic	2,4,10,100,500,1000,10000	1,2,5,7
15	Extended Powell	4,20,100,500,1000	2,4,6,8
16	Extended Denschnb	2,4,10,100,500,1000,10000	8,13,30,50
17	Hager	2,4,10,100	7,10,15,23
18	Extended Penalty	2,4,10,100	80,10,111,150
19	Quadrtic QF2	2,4,10,100,500,1000	5,20,50,100
20	Extended Quadratic Penalty QP2	2,4,10,100,500,1000	10,20,30,50
21	Extended Beale	2,4,10,100,500,1000,10000	-1,3,7,10
22	Diagonal 2	2,4,10,100,500,1000	1,5,10,15
23	Raydan1	2,4,10,100	1,3,7,10
24	Sum Squares	2,4,10,100,500,1000	1,3,7,10
25	Generlized Tridiagonal2	2, 4, 10, 100	15,18,20,22
26	Quadratic QF1	2, 4, 10,100, 500, 1000	3,5,8,10
27	Fletcher	4, 10, 100,500,1000,10000	3,5,8,9
28	Leon function	2	2,5,8,10
29	Extended Wood	4	3,5,20,30
30	Quartic function	4	5,10,15,20
31	Matyas function	2	1,5,10,15
32	Colville function	4	2,4,7,10

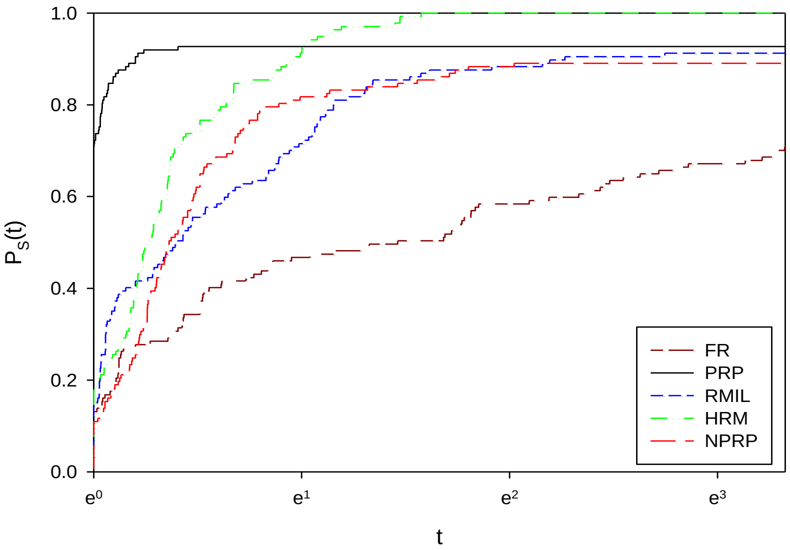

Figure 1: Performance profile relative to the number of iterations

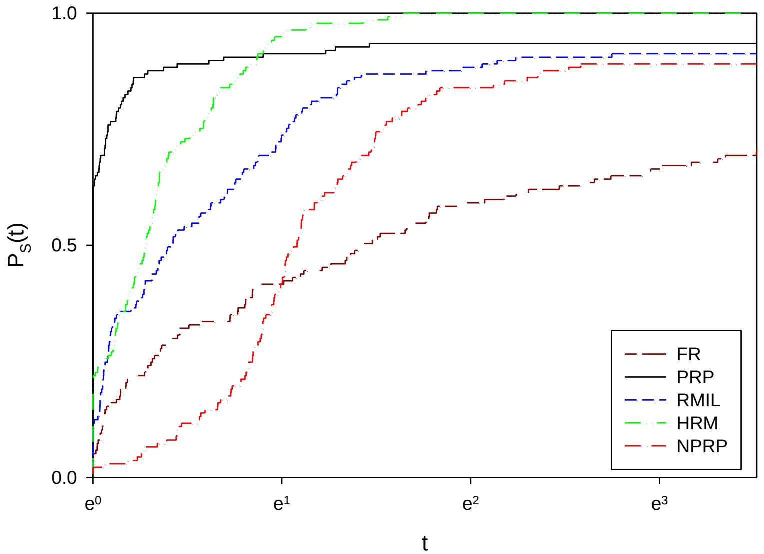

Figure 2: Performance profile relative to the CPU time

From figures 1-2 it is easy to see that the HRM method is the best among the four methods in the perspectives of the number of iterations and the CPU time. The PRP, $RMIL$ and $NPRP$ methods are much better than FR method, where the method PRP is preferable to the $RMIL$ method,and also, the $RMIL$ method is preferable to the $NPRP$ method, that is PRP can solve 93% of the problems, $RMIL$ can solve 91% of the problems, $NPRP$ can solve 89% of the problems and FR solved only 70%. Hence our new method successfully solved all the test problems,and it is competitive among the well-known conjugate gradient methods for unconstrained optimization.

5. CONCLUSION

In this paper, we propose a new β_k for unconstrained optimization, we prove that it is a global convergence with exact line search, and come out with best numerical results to illustrate their efficiency.

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