A New Modification of Nonlinear Conjugate Gradient Coefficients with Global Convergence Properties

Ahmad Alhawarat, Mustafa Mamat, Mohd Rivaie, Ismail Mohd

Abstract—Conjugate Gradient (CG) method has been enormously used to solve large scale unconstrained optimization problems due to the number of iteration, memory, CPU time, and convergence property. In this paper we proposed a new class of nonlinear conjugate gradient coefficient with global convergence properties proved by exact line search. The numerical results for our CG method new present an efficient numerical result when it compared with well-known formulas.

Keywords—Conjugate gradient method, conjugate gradient coefficient, global convergence.

I. INTRODUCTION

Nonlinear conjugate gradient method (CG) is useful method to find the minimum value of function for unconstrained optimization problems. Let us consider the following form:

\[ \min\{f(x) \mid x \in \mathbb{R}^n\}, \quad (1) \]

where \( f : \mathbb{R}^n \to \mathbb{R} \) is continuously differentiable and its gradient is denoted by \( g(x) = \nabla f(x) \), the method to find a sequence of points \( \{x_k\} \) starting from initial point \( \{x \in \mathbb{R}^n\} \) is given by iterative formula:

\[ x_{k+1} = x_k + \alpha_k d_k, \quad k = 0, 1, 2, 3, \ldots, \quad (2) \]

where \( x_k \) is the current iteration point and \( \alpha > 0 \) is the step size obtained by some line search. In this paper we used exact line search which is,

\[ f(x_k + \alpha_k d_k) = \min f(x_k + \alpha d_k), \alpha \geq 0. \quad (3) \]

Many researchers do not prefer to study this method, because it is very slow especially when the initial point is far away from the optimal solution point, so it is very expensive when compared with inexact line search, but our formula gives a good numerical result by using fast computer processors which is an advantage for exact line search method.

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

\[ d_k = \begin{cases} -g_k, & \text{if } k = 0, \\ -g_k + \beta_k d_{k-1}, & \text{if } k \geq 1, \end{cases} \quad (4) \]

where \( g_k = g(x_k) \) and \( \beta_k \) is scalar known as the conjugate gradient coefficient. The most well know formulas for \( \beta_k \) are as follows: (Hestenes–Stiefel (HS) [1]), (Fletcher–Reeves (FR) [2]), (Polak-Ribiere–Polyak (PR) [3]), (Conjugate Descent (CD) [4]), (Liu–Storey (LS) [5]), (Dai–Yuan (DY) [6]), (Wei et al. (WYL) [7]). (Mohd Rivaie, Mustafa Mamat, Ismail Mohd (RMIL) [17]).

\[ \beta_k^{FR} = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}}, \]
\[ \beta_k^{PRP} = \frac{g_k^T (g_k - g_{k-1})}{g_{k-1}^T g_{k-1}}, \]
\[ \beta_k^{CD} = -\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}}, \]
\[ \beta_k^{HS} = \frac{g_{k+1}^T (g_{k+1} - g_k)}{d_k^T (g_{k+1} - g_k)}, \]
\[ \beta_k^{DY} = \frac{g_k^T g_k}{(g_k - g_{k-1})^T d_{k-1}}, \]
\[ \beta_k^{RMIL} = \frac{g_k^T g_k}{\|d_{k-1}\|^2}. \]

The global convergence of FR method with exact line search was achieved by [8]; its behavior on numerical

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computation is unpredictable. Sometimes it is as efficient as PRP method, nevertheless most time it is very slow, also DY and CD have the same performance with exact line search.

Global convergence of PRP method for convex objective function under exact line search was proved by Polak and Ribiere in 1969 [3], in the other hand Powell gave out a counter example which shows that there exist non convex function, which PRP method does not converge globally even though the exact line search is used. After that Powell 1986 suggested that it is very important to achieve the global convergence of \( \beta_k \) should not be negative. Gilbert and Nocedal [9] proved that nonnegative PRP method is globally convergent with the Wolfe-Powel line search, before we start we need to simplify for exact line search easy to know if \( g_k^T d_k \geq c \) then stop. Otherwise go to Step2 with \( k = k + 1 \)

III. CONVERGENT ANALYSIS OF AMR* METHOD

In this section, the convergent properties of \( \beta_k^{AMR*} \) is studied, for above algorithm to be convergent, it should have fulfilled the sufficient descent condition and the global convergence properties.

A. Sufficient Descent Condition

For the sufficient descent condition to hold,

\[
g_k^T d_k \leq -c \| g_k \|^2 , \quad k \geq 0 \text{ and } c > 0 .
\]

Theorem 1. Consider a CG method with the search direction \( g_k^T d_k \geq c \| g_k \|^2 , \text{ for } k \geq 0 \text{ and } c > 0 .

Proof. From (4) we have if \( k = 0 \), the \( g_0^T d_0 = -c \| g_0 \|^2 \). for \( k \geq 1 \), we need to multiply (4) by \( g_{k+1}^T \) and set \( k = k + 1 \) then we have,

\[
g_{k+1}^T d_{k+1} = g_{k+1}^T (-g_{k+1} + \beta_k d_k) = -\| g_{k+1} \|^2 + \beta_k g_{k+1}^T d_k .
\]

for exact line search easy to know \( g_{k+1}^T d_k = 0 \). Thus

\[
g_{k+1}^T d_{k+1} = -\| g_{k+1} \|^2 .
\]

Thus, sufficient descent direction holds. The proof is completed.

B. Global Convergence Properties

We need to show that \( \beta_k^{AMR*} \) is globally convergent under exact line search, before we start we need to simplify \( \beta_k^{AMR*} \) to

\[
\beta_k^{AMR*} = \frac{g_k^T (m \| g_k \| - g_{k+1})}{\| g_k\| \| g_k - g_{k+1} \|},
\]

where \( m = \| g_{k+1} \| / \| g_k \| \), and \( \|g\| \) means the Euclidean norm.
\[ \beta_k^{4MR} = \frac{g_k^T (g_{k-1} - g_k)}{g_{k-1}^T (g_{k-1} - g_k)} \geq \frac{\|g_k\| \|g_{k-1}\| - \|g_k - g_{k-1}\|}{\|g_{k-1}\|} = 0. \]  

Thus we get

\[ \beta_k^{4MR} \geq 0. \]  

and,

\[ \beta_k^{4MR} = \frac{g_k^T (g_{k-1} - g_k)}{g_{k-1}^T (g_{k-1} - g_k)} \leq \frac{\|g_k\|^2 + \|g_{k-1}\|^2}{\|g_{k-1}\|^2} \leq \frac{2\|g_k\|^2}{\|g_{k-1}\|^2} \]

which implies

\[ \beta_k^{4MR} \leq \frac{2\|g_k\|^2}{\|g_{k-1}\|^2}. \]  

The following assumptions are needed to use in our proof.

**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 and \( \Omega \) is bounded.

**Assumption B.** In some neighborhood \( N \) of \( \Omega \), \( f \) is continues and differentiable, and its gradient is Lipchitz continues, that is, for any \( x, y \in \mathbb{R}^n \), there exists a constant \( L \geq 0 \) such that:

\[ \|g(x) - g(y)\| \leq L\|x - y\|. \]

Under the above assumptions, we have the following Lemma:

**Lemma 1.** Suppose the Assumptions A and B hold true, consider any form of (4), for all \( k \) and \( \alpha_k \) satisfied (3) the following condition, known as the Zoutendijk condition holds

\[ \sum_{k=0}^{\infty} \|g_kd_k\|^2 < \infty, \]

the proof of this Lemma can be seen [8].

By substitute (8) in Zoutendijk condition then it is equivalent to,

\[ \sum_{k=0}^{\infty} \|\alpha_k d_k\|^2 < \infty. \]  

\[ \liminf \|g_k\| = 0. \]  

**Proof.** We use proof by contradiction, firstly consider \( \theta_k \) is the angle between \( d_k \) and the steepest descent search direction \( -g_k \), where

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

By using (4) and (15) we indicate the following relations,

\[ \|d_k\| = \sec \theta_k \|g_k\| \]

\[ \beta_k = \|d_k\| = \tan \theta_{k-1} \|g_{k-1}\| \]

Combining (16) and (17), indicate

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

\[ \tan \theta_{k+1} = \frac{\|g_{k+1}\|^2}{\|g_{k+1}\|^2} \sec \theta_k \]

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Suppose (14) does not hold true, then for all \( k \), there exist \( \varepsilon > 0 \), such that

\[ \|g_k\| \geq \varepsilon \]  

By \( \|x_{k+1} - x_k\| \rightarrow 0 \) and Lipschitz condition

\[ \|g_{k+1} - g_k\| \leq \varepsilon. \]

Since

\[ \|g_{k+1} - g_k\| = \|g_{k+1} - g_k\|. \]

This imply that
\[ |g_{k+1}| \leq 2 \varepsilon. \]

So
\[ \tan \theta_{k+1} \leq 4 \sec \theta_k. \]

Since \( \sec \theta_k \geq \tan \theta_k \), for all \( \theta_k \in [0, \frac{\pi}{2}) \), we have \( \tan \theta_{k+1} \leq 4 \tan \theta_k \).

Therefore the angle between \( d_k \) and the steepest descent direction \( -g_k \) is bounded away from \( \frac{\pi}{2} \), so from (11), (12), and (17) we have,
\[
\sum_{i=0}^{\infty} \frac{\|g_{k+1}\|^{1/2}}{\|d_k\|^{1/2}} = \sum_{i=0}^{\infty} \|g_k\|^2 (\cos \theta_k)^2 < \infty
\]

This implies \( \lim_{k \to \infty} \|g_k\| = 0 \), which contradicts (14). The proof is complete.

D. Linear Convergence Rate

In this section, we shall discuss linear convergence rate for AMR* method under this convergence, we need the following necessary assumption to prove.

Assumption C. The sequence (2) where \( \alpha_k \) generated by the exact line search \( d_k \) and \( \beta_k \) generated by (4) and (5) respectively, converges to \( x^* \). In addition, \( \nabla^2 f(x^*) \) is a symmetric positive definite matrix and twice continuously differentiable on \( N(x^*, \varepsilon) \).

The conclusion of the following Lemma is used to prove the linear convergence of nonlinear conjugate gradient methods. The proof can be seen given in [18], [19].

Lemma 2. If Assumption 2 holds true, then \( m, M \) and \( \varepsilon_1 \) exist with \( 0 < m \leq M \) and \( \varepsilon < \varepsilon_1 \) such that,
\[
m \|y\|^2 \leq y^T \nabla^2 f(x) y \leq M \|y\|^2
\]
for all \( x, y \in N(x^*, \varepsilon) \),
\[
\frac{1}{2} m \|x - x^*\|^2 \leq f(x) - f(x^*) \leq \frac{1}{2} M \|x - x^*\|^2
\]
for all \( x, x^* \in N(x^*, \varepsilon) \),
\[
m \|x - y\|^2 \leq (g(x) - g(y))^T (x - y) \leq M \|x - y\|^2
\]
for all \( x, y \in N(x^*, \varepsilon) \). (20)

Thus we get
\[
m \|x - y\|^2 \leq g(x)^T (x - x^*) \leq M \|x - x^*\|^2
\]
for all \( x \in N(x^*, \varepsilon) \). (21)

Using Cauchy–Schwartz inequality, (20) and (21) we obtain
\[
m \|x - x^*\| \leq \|g(x)\| \leq M \|x - x^*\|
\]
for all \( x, y \in N(x^*, \varepsilon) \).

and
\[
\|g(x) - g(y)\| \leq M \|x - x^*\|
\]
for all \( x, y \in N(x^*, \varepsilon) \).

Lemma 3. Supposed Assumption C holds true, and let \( \theta_k \) be the angle between \( -g_k \) and \( d_k \), the sequence \( x_k \) is generated by the exact line search and \( d_k \) is a descent direction. If a constant \( \eta > 0 \) exist for which,
\[
\prod_{i=0}^{k+1} \cos \theta_i \geq \eta^k
\]
then a constant \( a > 0 \) and \( r \in (0,1) \) exist, such that
\[
\|x_{k+1} - x^*\| \leq ar^{k+1}.
\]

Hence \( x_k \) will converge to \( x^* \) at least R-linearly. The proof for this Lemma can be seen from [20].

Theorem 5. If Assumption C holds true, then constants \( \alpha > 0 \) and \( \mu \) exist such that the sequence generated by (2), (4) and (1) using the exact line search satisfies,
\[
\|x_{k+1} - x^*\| \leq \alpha r^{k+1},
\]
hence, \( x_k \) will converge to \( x^* \) at least R-linearly.

Proof. If Assumption C hold true, then we assume, \( \forall x_0 \in N(x^*, \varepsilon) \), therefore from (4) and (10) we indicate
\[
\|d_k\| \leq \|g_k\| + \beta_k \|d_{k-1}\| \leq \|g_k\| + \|g_k\| \leq \|d_{k-1}\| \leq \left(1 + \frac{2}{\|g_k\|}\right) \|d_k\|
\]
thus,
\[
\cos \theta_k = \frac{-g_k^T d_k}{\|g_k\| \|d_k\|} = \frac{\|g_k\|^2}{\|g_k\| \|d_k\|} \geq \left(1 + \frac{2}{\|g_k\|}\right)^{-1} > 0
\]
Hence, Lemma 3 holds true. By (22) we can obtain (23). The proof is completed.

IV. NUMERICAL RESULTS AND DISCUSSIONS

In this section, we use some test problems to find the computational results to analyze the efficiency of AMR*. We
performed a comparison with other CG methods, including PR and WYL. The tolerance $\varepsilon$ is selected as equal to $10^{-5}$ for all algorithms to investigate how rapidly the iteration of these algorithms converge towards the optimal solution, also the gradient value of the stopping criteria. Hence the stopping criteria are set $\|g_k\| \leq 10^{-5}$, the test functions can be found on many trusted web sites with a lot of codes for exact and inexact line search made by Fortran, Matlab, C, and C++, Hager and Andrei as an example and others. We used Maple 13 subroutine program, with CPU processor Intel (R) Core (TM), i7 CPU, and 4GB RAM memory. The performance results are shown in Figs. 1 and 2, respectively, using a performance profile introduced by Dolan and More [20]. In this performance profile, they introduced the notion of a means to evaluate and compare the performance of the solver $s$ on a test set $P$. Assuming $n_s$ solvers and $n_p$ problems exists for each problem $P$ and solver $S$, they define $\tau_{p,s} = \text{time (number of iterations or CPU time or others)}$ required to solve problems $P$ by solver $S$.

Requiring a baseline for comparisons, they compared the performance on problem $P$ by solver $S$ with the best performance of any solver on this problem using the performance ratio

$$\rho_s(t) = \frac{1}{n_p} \min_{p \in P} \{ \tau_{p,s} \}$$

Thus $\rho_s(t)$ was the probability for solver $s \in S$ that a performance ratio $\tau_{p,s}$ was within a factor $t \in R$ of the best possible ratio, function $P_s$ was the cumulative distribution function for performance ratio, the performance profile $p_s : R \rightarrow [0,1]$ for a solver was a non-decreasing piecewise, and continuous from the right. The value of $\rho_s(t)$ is the probability that the solver will win over the rest of the solvers. In general, a solver with high values of $p(t)$ or at the top right of the figure are preferable or represent the best solver.

Figs. 1 and 2 show that AMR* is best performance, since it can solve all test problems and reach 100%. Although the performance of PRP seems to be much better than AMR*, but it can solve only 90% and WYL solved 87% and it seems less than AMR* for both performance. Hence we considered AMR* as the best and superior method above since that can solve all problems.

V. CONCLUSION

In this paper, we have proposed a new and simple $\beta$ that is easy to implement. Our numerical results have shown that, our new method has the best performance compared to the other standard CG methods. We have also provide proof showing that this method converges globally with a linear convergence rate, in future we intend to test $\beta^{AMR}$ using inexact line search under strong Wolf condition, Armijo line search and Grippo-Lucidi line search, also we can make some modification to improve $\beta^{AMR}$ to get results characterized by speed, accuracy, and less space in memory using various types line search.

<table>
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<tr>
<th>No.</th>
<th>Function</th>
<th>Number of variables</th>
<th>Initial points</th>
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REFERENCES