New Conjugate Gradient Method Addressing Large Scale Unconstrained Optimization Problem

Ummie Khalthum Mohd Yusof, Mohd Asrul Hery Ibrahim, Mohd Rivaie, Mustafa Mamat, Mohamad Afendee Mohamed, Puspa Liza Ghazali

Abstract—An iterative conjugate gradient (CG) method is prominently known for dealing with unconstrained optimization problem. A new CG method which is modified by Wei Yao Liu (WYL) method is tested by standard test functions. Moreover, the step size is calculated using exact line search. Theoretical proofs on convergence analysis are shown. As a result, this new CG is comparable to the other methods in finding the optimal points by measuring the total iterations required as well as the computing time. Numerical results showed the execution between three CG methods in details.

Index Terms: Conjugate gradient (CG) method, global convergence, sufficient descent condition, unconstrained optimization.

I. INTRODUCTION

The conjugate gradient (CG) algorithm is an iterative method for unconstrained minimization that produces more appropriate approximation to the minimum of general unconstrained nonlinear problems at each iteration. The main advantages of this method is capable to solve large scale problems since it not necessitate to construct and store any matrix. Due to accomplish objective function, the performance of the conjugate coefficient plays an important role. Starting in 1952, Hestenes-Stiefel develop this method by introduce conjugate coefficient namely \( \beta^H \) method, then continues with \( \beta^F \) by Fletcher-Reeves in 1965. Then, Polak-Ribiere introduced new alteration in 1969 as \( \beta^P \) [1]. However \( \beta^F \) is the most efficient among the class of conjugate directions methods. All the modification in this method based on conjugate coefficient, \( \beta \). Recently, researchers keep develop their own \( \beta \) based on ideas from previous and make comparison in terms of their performance. In most recent studies, this method are simple and easy to implement compare Newton method because of Hessian matrix need more time consuming to perform [13], [20], [21]. Recent development, researchers come out with much effort to design and construct another model for CG methods which produce excellent numerical achievements that satisfy global convergence properties.

The objective function for unconstrained optimization problems is denoted as

\[
\min_{x \in \mathbb{R}^n} f(x) \tag{1}
\]

where \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) is continuously differentiable over \( n \) dimensional Euclidean space. To solve (1), we use iterative method termed as,

\[
x_{k+1} = x_k + \alpha_k d_k \tag{2}
\]

with \( x_{k+1}, \alpha_k, d_k \) are new iterate point, step size and search direction respectively. In (3), we found the search direction

\[
d_k = \begin{cases} 
- \frac{g_k}{g_k^T g_{k-1}} & \text{if } k = 0 \\
- \frac{g_k + \beta_k d_{k-1}}{g_{k-1}^T g_{k-1}} & \text{if } k \geq 1 
\end{cases} \tag{3}
\]

with \( g_k \) is a \( f(x) \) gradient at \( x_k \) while \( \beta_k \) is CG coefficient.

Previous studies gives valuable intentions to latest researchers come out with new CG coefficient that gain ideas from the classical \( \beta \) as listed in Table 1.

<table>
<thead>
<tr>
<th>Table 1: CG coefficients</th>
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<tr>
<td>CG Coefficients</td>
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<tr>
<td>( \beta^H )</td>
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<tr>
<td>( \beta^F )</td>
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<td>( \beta^P )</td>
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Nowadays, many researchers develop new formula and some commonly used and also widely known are [2], [5], [6], [12], [15], [17]-[19], [23].

Line search is a technique to calculate the step size, \( \alpha \), along a given search direction \( d_k \).

To determine the values of the step size, either exact or inexact line search can be used. Armijo is the first method in inexact and followed by Goldstein, Wolfe and Strong Wolfe method. The ways to find \( \alpha \) will effects both the convergence and the speed of convergence of the algorithm. However, this paper only studied CG algorithms with exact line search,
\[ \min_{x \in \mathbb{R}^n} f(x + \alpha_i d_i) \quad (4) \]

II. THE NEW COEFFICIENT

A. Propose New Coefficient

In this study, a new CG method with namely \(\beta^{UAM}_k\) (Ummie, Asrul and Mustafa) proposed by pursuing the excellent performance of coefficient proposed by [22], [7] in term of successful to solve the test problem.

Hence, the complete algorithms for the CG methods are arranged by the following pseudo-code,

1. Set \(k\) to 0 with initial point, \(x_0\) an element of \(\mathbb{R}^n\)
2. Compute \(\beta_k\) as (5)
3. Calculate the \(d_k\) using (3). If \(\|g_k\| = 0\), then exit.
4. Compute the \(\alpha_k\) by (4)
5. Compute \(x_{k+1}\) based on (2)
6. Evaluate convergence property, followed by stopping condition such that if \(f(x_{k+1}) < f(x_k)\) and \(\|g_{k+1}\| \leq \varepsilon\), then exit. Else, jump to step 1 and increase \(k\) by one.

B. Convergence Analysis

The convergence analysis of \(\beta^{UAM}_k\) are presented. Furthermore, we establish the sufficient descent condition and global convergent to ensure an algorithm satisfy both conditions.

C. Sufficient Descent Condition

For \(k \geq 0\), each \(d_k\) should satisfy the descent condition by the following assumption

\[ g_k^T d_k < 0 \quad (6) \]

Suppose there exists a constant, \(c_1 > 0\), then

\[ 0 \leq \varepsilon \|g_k\| \quad (7) \]

which dictates the fulfillment of this condition by search direction.

Theorem 1. Assume CG method as in (5), search direction as (3) with the condition (7) also hold for \(k \geq 0\).

Proof. If \(k \geq 0\) then we get (7). When \(k \geq 1\), we prove by induction. By multiplying our search direction (3) with \(g_k^T\), we get,

\[ g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 + \beta^{UAM}_k g_k^T d_k \]

For exact line search, \(g_k^T d_k = 0\). Hence \(g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2\). Thus, sufficient descent direction holds and completes the proof.

D. Global Convergence Properties

In making sure there are remain not less than zero to examine the global convergence properties, \(\beta^{UAM}_k\) is simplified as follow:

\[ \beta^{UAM}_k = \max \left\{ 0, \frac{g_k^T \left( g_{k+1} - \frac{\|g_k\|}{\|g_{k+1}\|} g_{k+1} \right) g_k}{\|g_k\|^2} \right\} \quad (5) \]

Thus,

\[ 0 \leq \beta^{UAM}_k \leq \frac{\|g_{k+1}\|^2}{\|g_k\|^2} \quad (8) \]

In studying of global convergence properties, the following assumptions are deemed necessary.

Assumption 1

1) At the initial point \(x_0\), \(f\) is bounded below objective function and is continuously differentiable on \(\mathbb{R}\) for some neighborhood \(N\).

2) For \(f\) having gradient \(g(x)\) given by Lipschitz continuous in \(N\), then for any given constant \(L > 0\), the expression \(\|g(x) - g(y)\| \leq L \|x - y\|\) holds for any \(x, y \in N\).

From here, we reserve to the subsequent lemma (Zoutendijk).

Lemma 1. Let Assumption 1 be true. An iterative CG scheme having search direction \(d_k\) as well as step size \(\alpha_k\) fulfils the exact line search. Consequently, Zoutendijk condition holds such that

\[ \sum_{\tau=1}^{\infty} \frac{\sum_{\tau=1}^{\infty} (g_k^\tau d_k^\tau)^2}{\|d_k\|^2} < \infty \quad (10) \]

Proof. Theorem 2 is verified by contradiction. If incorrect, then a constant \(c > 0\) holds, whereas \(\|g_{k+1}\| \geq c\) (11)

Claiming (3) and squaring both sides, we come to

\[ \|d_{k+1}\|^2 = (\beta^{UAM}_{k+1})^\tau \|d_k\|^2 - 2 \beta^{UAM}_{k+1} g_{k+1}^\tau d_{k+1} - \|g_{k+1}\|^2 \quad (12) \]

Consuming \(g_{k+1}^\tau d_{k+1}\) and dividing both sides,

\[ \|d_{k+1}\|^2 = (\beta^{UAM}_{k+1})^\tau \|d_k\|^2 - 2 \beta^{UAM}_{k+1} g_{k+1}^\tau d_{k+1} - \|g_{k+1}\|^2 \quad (13) \]

Completing the square,
Applying (7) results

\[
\left( \beta_{UAM}^{t+1} \right) \| d_t \|^2 \\
\leq \left( \beta_{UAM}^{t} \right) \| d_t \|^2 + \frac{1}{\| g_t \|} \left( \frac{1}{\| g_t \|} + \frac{1}{\| g_t \|} \right)\| d_t \|^2
\]

Therefore, it becomes

\[
\left( \beta_{UAM}^{t} \right) \| d_t \|^2 \leq \frac{1}{\| g_t \|} \left( \frac{1}{\| g_t \|} + \frac{1}{\| g_t \|} \right)\| d_t \|^2
\]

Since \( \beta_{UAM}^{t} \geq 0 \) it becomes

\[
\left( \beta_{UAM}^{t} \right) \| d_t \|^2 \leq \frac{1}{\| g_t \|} \left( \frac{1}{\| g_t \|} + \frac{1}{\| g_t \|} \right)\| d_t \|^2
\]

Therefore,

\[
\sum_{t=1}^{\infty} \left( \beta_{UAM}^{t} \right) \| d_t \|^2 = \infty
\]

However, it is contradictory to Lemma 1. Hence, condition (8) is true and the proof is concluded.

### III. RESULTS AND DISCUSSION

An overview numerical result from many different conjugate gradient methods gives various results in how performance profile looks. By using test problem based on Andrei [3], the methods are fully tested with dimension between 2 to 500 variables [14].

In total, we have 180 test problems where the initial points are subtracted from the minimum point. The stopping criteria, \( \| s_t \| \leq 0 \) if the iteration number exceeds the limit of 10,000.

The outcomes are displayed in Fig. 1 and 2 utilizing performance profile improved by [16]. The performance profile aims to show performance of the new coefficient in order to meet optimal solutions compared with another two coefficients. Regarding on Fig. 1, the \( \beta_{UAM}^{t} \) yields the best performance in terms of test problem solved with the fastest method. However, in Fig. 2, it can be summarized that \( \beta_{UAM}^{t} \) is as good as \( \beta^{t} \) at the starting movement, but by referring to the right hand side of graph, the percentage of test problem solved by the new method is the highest compared to others. In conclusion, it’s shown our coefficient is better and able to deal with the entire test problem [4].

### IV. CONCLUSION

A new coefficient, \( \beta_{UAM}^{t} \) with impressive performance is introduced in order to achieve optimal solutions. For the next interest, this new coefficient can be extended in hybrid between CG and BFGS methods with the search direction proposed by [8]-[11].

### V. ACKNOWLEDGMENT

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### REFERENCES

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