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Research paper

A Modification of Conjugate Gradient Method using Strong Wolfe Line Search

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Abstract

In this paper, a proposed modification of conjugate gradient (CG) coefficient β_k method to solve unconstrained optimization problems is presented. A strong - Wolfe line search is used to generate β_k with sufficient descent direction and global convergence property is established. Numerical result are also presented based on the number of iterations and CPU times, the results have shown that the modified β_k performs better compare to other CG methods.

Keywords: *Optimizations; Conjugate Gradient; Line Search.*

1. Introduction

The strength of the conjugate gradient (CG) methods are useful in finding the minimum value of a function for unconstrained optimization problem. The low memory storage also played an important role in the CG methods **[**10, 17**]**. Generally, for n number of variables function the method can be expressed in the form:

$$\min_{x\epsilon R^n} f(x) \tag{1}$$

where $f: R^n \to R$ is continuously differentiable function. The CG methods generates its update iteratively in the form.

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

where x_k is the current iteration point, $\alpha_k > 0$ is a positive step size and d_k is the search direction which is defined by

$$d_k = \begin{cases} -g_k \; for \; k = 0, \\ -g_k + \beta_k d_{k-1} \; for \; k \geq 1, \end{cases} \tag{3}$$

where g_k and β_k is the gradient and conjugate gradient coefficient of $f(x)$ respectively at the point x_k. Some well-known CG methods have been proposed by many researchers [1-5, 15] are given as follows:

$$\beta_k^{FR} = \frac{g_k^T g_k}{\|g_{K-1}\|^2}, \qquad \beta_k^{PR} = \frac{g_k^T (g_k - g_{k-1})}{\|g_{k-1}\|^2} \qquad \beta_k^{HS} = \frac{g_k^T (g_k - g_{k-1})}{(g_k - g_{k-1})^T d_{k-1}}, \tag{4}$$

$$\beta_k^{DY} = \frac{g_k^T g_k}{(g_k - g_{k-1})^T d_{k-1}}, \qquad \beta_k^{LS} = \frac{g_k^T (g_k - g_{k-1})}{- d_{k-1} g_{k-1}} \qquad \beta_k^{CD} = -\frac{g_k^T g_k}{(d_{k-1}^T g_{k-1})}$$

where g_k and g_{k-1} denote the gradient of $f(x)$ at the point x_k and x_{k-1} respectively. The conjugate gradient coefficient $\beta_k \in R$ is a scalar, which determine different CG methods. The above methods are known respectively as Fletcher and Reeve's (FR) [13], Polak and Ribiere (PR) [14], Hestenes and Steifel (HS) [6], Liu and Storey (LS) [11], Dai and Yuan (DY) [21], Conjugate Descent (CD) by Fletcher [13], Rivaie et al. [7], Ghani et al. [16] and Shoid et al. [18,]. There are several line search methods used, these includes Armijo [9], Wolfe [12] and Goldstein [19], their application in algorithm is to perform one-dimensional search to determine the value of the step size α_k. The applications of CG can be referred to [25-29].

In this study, we examined the results on the convergence using inexact line search method, the following strong – Wolfe condition is used:

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \rho \alpha_k {d_k}^T g_k \tag{5}$$

$$|g(x_k + \propto_k d_k)^T d_k| \leq -\sigma \, {d_k}^T g_k \tag{6}$$

with $0 < \rho < \sigma < 1$.

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Based on the numerical results obtained, β_k^{MMM} performs better than RMFI and FR CG methods. However, the sufficient descent and the global convergence is satisfying under strong – Wolfe condition. The formula satisfies the sufficient descent condition and has been proved to converge globally under Strong – Wolfe line search. The modification of RMFI method named MMM gives impressive and efficient results when compare with the classical RMFI conjugate gradient method. In the next section, we show the modified CG method and its algorithm. In Section 3, we present the numerical result and discussions.

2. Modified Conjugate Gradient Method

In this section, a modified formula for unconstrained (CG) named as β_k^{MMM} is presented. The MMM refer to the researcher's name Mandara, Mustafa and Mohammad. This β_k is a modification based on RMFI and FR methods. The modified β_k is substantial and is defined by

$$\beta_k^{MMM} = \frac{g_k^T g_k}{{d_{k-1}}^T(d_{k-1}-g_k)} = \frac{\|g_k\|}{{d_{k-1}}^T(d_{k-1}-g_k)} \tag{7}$$

where $\|g_k\|$ denotes the Euclidean norm of vectors.

Algorithm 1

The following is the algorithm for β_k^{MMM}.

Step 1: Given x_0, set $k = 0$.

Step 2: Compute β_k based on β_k^{MMM} as in (7).

Step 3: Compute search direction d_k using in (3). If $\|g_k\| = 0$, then stop. Otherwise, continues with step 4.

Step 4: Compute step size α_k such that

$$f(x_k + \alpha_k d_k) \le f(x_k) + \rho\alpha_k {d_k}^T g_k$$
$$|g(x_k + \alpha_k d_k)^T d_k| \le -\sigma\, {d_k}^T g_k$$

Step 5: Update new point via $x_{k+1} = x_k + \alpha_k d_k$.

Step 6: Compute $f(x_{k+1}) < f(x_k)$ and $\|g_k\| \le \epsilon$, then stop. Otherwise, go to step 1 with $k = k + 1$.

3. Convergence Analysis

The convergence properties of β_k^{MMM} is studied and presented. First, the sufficient condition is established, there exists a constant $c > 0$ for all $k \ge 0$. Then, the search directions will satisfy the sufficiently descent condition.

$$g_k^T d_k \le -c\|g_k\|^2 \tag{8}$$

Theorem 1: Suppose that the sequence g_k and d_k are generated by the Algorithm 1, and the step length is determined by strong - Wolfe line search in (5) and (6). If $\sigma < \frac{1}{5}$, then the sequence d_k satisfy the sufficient descent condition in (8).

Proof

By applying in (7), we have

$$\beta_k^{MMM} = \frac{g_k^T g_k}{{d_{k-1}}^T(d_{k-1}-g_k)} = \frac{\|g_k\|^2}{\|d_{k-1}\|^2 - {d_{k-1}}^T g_k} \le \frac{\|g_k\|^2}{\|d_{k-1}\|^2} \tag{9}$$

with $\|g_k\|$ as the Euclidean norm of vectors. By using in (3), we have

$$\frac{g_{k+1}^T d_{k-1}}{\|g_{k+1}\|^2} = -1 + \beta_k^{MMM}\frac{g_{k+1}^T d_k}{\|g_{k+1}\|^2} \tag{10}$$

Using induction, the descent property is shown since $g_0^T d_0 = -\|g_0\|^2 < 0 \ and \ g_0 \ne 0.$

Suppose $d_i, i = 1, 2, 3, \cdots, k.$ are all descent direction. By using in (6) and inequalities in (9), the following is obtained.

$$\beta_k^{MMM}|g_{k+1}^T d_k| \le \frac{\|g_k\|^2}{\|d_{k-1}\|^2}\,\sigma(-g_k^T d_k)$$

$$\sigma\frac{\|g_k\|^2}{\|d_{k-1}\|^2}(g_k^T d_k) \le \beta_k^{MMM} g_{k+1}^T d_k \le -\sigma\frac{\|g_k\|^2}{\|d_{k-1}\|^2}(g_k^T d_k) \tag{11}$$

Also, in (10) and (11), we deduce that:

$$-1 + \sigma\frac{g_k^T d_k}{\|d_{k-1}\|^2} \le \frac{g_{k+1}^T d_k}{\|g_{k+1}\|^2} \le -1 - \sigma\frac{g_k^T d_k}{\|d_{k-1}\|^2}. \tag{12}$$

Repeating the process and since $g_0^T d_0 = -\|g_0\|^2$, this imply

$$-1 + \sigma(-1) \le \frac{g_0^T d_0}{\|g_0\|^2} \le -1 - \sigma(-1) \tag{13}$$
$$-1 - \sum_{i=1}^k \sigma^i \le \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \le -1 + \sum_{i=1}^k \sigma^i \tag{14}$$
$$-1 - \sum_{i=1}^k \sigma^i \le \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \le -2 + 1 + \sum_{i=1}^k \sigma^i \tag{15}$$
$$-\sum_{i=0}^k \sigma^i \le \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \le -2 + \sum_{i=1}^k \sigma^i \tag{16}$$

Since,

$$\sum_{i=0}^k [\sigma]^i < \sum_{i=0}^\infty [\sigma]^i = \frac{1}{1-\sigma}. \tag{17}$$

Then, in (16) can be written as

$$-\frac{1}{1-\sigma} \le \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \le -2 + \frac{1}{1-\sigma}. \tag{18}$$

Therefore, by applying the method of induction $g_k^T d_k < 0$ holds for all k ≥ 0.

Let c$= 2 - \frac{1}{1-\sigma}$ where $c \in (0,1)$, then

$$c - 2 \le \frac{g_{k+1}^T d_{k+1}}{\|g_{k+1}\|^2} \le -c. \tag{19}$$

Thus, the proof is complete.

The proof of global convergence, the following assumption is considered.

Assumption 1

i) $f(x)$ has lower bound, on the level set $\ell = \{x|f(x) \le f(x_0)\}$ where x_0 is the starting point [8].

ii) In a neighborhood N of ℓ, the function $f(x)$ is continuously differentiable and its gradient is Lipschitz continuous; then there exists a constant L > o such that $\|g(x) - g(y)\| \le L\|x - y\|$, for all x, y $\in N$. [20]. Based on Assumption 1, the following lemma by [24] to verify the Global convergence of the above method is used.

Lemma 1: Suppose that Assumption 1 holds true. Let the sequence $\{g_k\}$ and $\{d_k\}$ be generated by algorithm 1, and the step length

is determined by the strong - Wolfe line search in (5) and (6). Then, the condition known as Zoutendijk [24] holds.

$$\sum_{k=0}^{\infty} \frac{\left(g_k^T d_k\right)^2}{\|d_k\|^2} < +\infty. \quad (20)$$

Theorem 2: Suppose that Assumption 1 holds true. Let the sequence $\{g_k\}$ and $\{d_k\}$ are generated by algorithm 1 and α_k is determined by the Strong – Wolfe line search in (5) and (6), the sufficient descent condition hold true. Then,

$$\lim_{k\to\infty} inf\|g_k\| = 0. \quad (21)$$

Proof: In (6), (8) and the Zoutendijk condition in (20), we obtained

$$\sum_{k=0}^{\infty} \frac{\|g_k\|^4}{\|d_k\|^2} < +\infty. \quad (22)$$

Now, let $m_k = \frac{\|d_k\|^2}{\|g_k\|^4}$. (23)

So, in (22) can be re-written as

$$\sum_{k=0}^{\infty} \frac{1}{m_k} < +\infty. \quad (24)$$

Using the concept of prove by contradiction, this is carried out by assuming that theorem 2 is not true, then there exist a positive constant p > 0 such that

$$\|g_k\| \geq p, \text{ for all } k \geq 0\,. \quad (25)$$

Re-writing in (3) as

$$d_k + g_k = \beta_k^{MMM} d_{k-1} \quad (26)$$

Squaring both sides in (26), we obtain

$$\|d_k\|^2 = (\beta_k^{MMM})^2\|d_{k-1}\|^2 - 2g_k^T d_k - \|g_k\|^2. \quad (27)$$

$$\|d_k\|^2 = \left(\frac{\|g_k\|^2}{\|d_{k-1}\|^2}\right)^2 \|d_{k-1}\|^2 - 2g_k^T d_k - \|g_k\|^2$$

$$\|d_k\|^2 = \frac{\|g_k\|^4}{\|d_{k-1}\|^2} - 2g_k^T d_k - \|g_k\|^2$$

Dividing both side by $\|g_k\|^4$, and applying in (9) and (24), we get

$$m_k \leq \frac{1}{\|d_{k-1}\|^2} - \left(2\frac{\left|g_k^T d_k\right|}{\|g_k\|^2} - 1\right)\frac{1}{\|g_k\|^2} \leq \frac{1}{\|d_{k-1}\|^2}. \quad (28)$$

Table 1: List of problem functions

Hence,

$$m_k \leq \sum_{i=0}^{k} \frac{1}{\|d_i\|} \quad (29)$$

$$\frac{1}{m_k} \geq \frac{p^2}{k} \quad (30)$$

Thus, in (28) and (24), it follows that

$$\sum_{i=0}^{\infty} \frac{1}{m_k} = +\infty, \quad (31)$$

which contradicts the condition (25). Therefore, this proves the theorem.

4. Results and Discussion

This section cover the numerical results of β_k^{MMM} using Algorithm 1. The result is compared with the other CG methods for unconstrained optimization, using different test functions. The result for modification of the proposed method β_k^{MMM} are compared to RMFI [7] and FR [13] methods under Strong-Wolfe line search. These three methods have been tested using several test functions problems with four different initial points. The output is based on number of iterations and CPU time. Considering $\epsilon = 10^{-6}$, all the methods are terminated when the stopping criteria $\|g_k\| \leq 10^{-6}$ is fulfilled. We used MATLAB R2012b and run using Intel Core i5 with RAM 2GB and Window 7 Operation System. Table 1 presents a list of problem functions, dimension and the initial points to test the proposed method.

Table 1: The serial number of a given test problems, list of named functions, dimensions and initial points of all functions used.

No.	Functions	Dimensions	Initial Points
1	Trecanni	2	(2,…,2), (11,…,11), (17,…, 17), (-17,…,-17)
2	Booth	2	(4,…,4), (-4,…,-4), (7,…,7), (9,…,9)
3	Three Hump Camel	2	(3,…,3), (-3,…,-3), (7,…,7), (51,…,51)
4	Six Hump Camel	2	(11,…,11), (21,…,21), (31,…,31), (41,…,41)
5	Zettl	2	(-3,…,-3), (5,…,5), (7,…,7), (13,…,13)
6	Leon	2	(2,…,2), (4,…,4), (13,…,13), (-13,…,-13)
7	Colville	4	(-2,-2,…,-2), (4,4,…,4), (7,7,…,7), (9,9,…,9)
8	Wood	4	(-21,-21,…-21), (13,13,…,13), (9,9,…,9), (-17,-17,…,-17).
9	Gen. Tridiagonal 1	10	(7,7,…,7), (-7,-7,…-7),(14,14,…,14),(-14,-14,…14)
10	Gen. Tridiagonal 2	10	(3,3,…,3), (5,5,…,5), (7,7,…,7), (12,12,…,12).
11	Fletcher	10	(7,7,…,7), (5,5,…,5), (3,3,…,3), (2,2,…,2).
12	Hager	100	(2,2,…,2),(5,5,…,5),(7,7,…,7),(10,10,…,10).
13	Raydan	100	(-3,-3,…,-3), (-5,-5,…,-5), (-8,-8,…,-8), (-11,-11,…,-11)
14	Dixon and Price	100	(-42,-42,…,-42), (-49,-49,…,-49),(-81,-81,….,-81), (-99,-99,…,-99).
15	Quadratic. QP1	100	(-11,-11,…,-11), (-40,-40,…,-40), (-49,-49,…,-49), (49,49,…,49).
16	Quadratic. QP2	100	(5,5,…,5), (-5,-5,…,-5), (11,11,…,11), (-11,-11,…,-11)
17	Extended Penalty	100	(50,50,…,50),(100,100,…,100),(200,200,…,200), (-50,-50,…,-50).
18	Extended Maratos	100	(2,2,…,2), (5,5,…,5), (25,25,…,25), (49,49,…,49)
19	Quadratic QF2	100	(80,80,…,80), (100,100,…,100),(200,200,…,200), (-200,-200,…,-200).
20	Extended Tridiagonal 1	100, 1000	(10,10,…,10), (-10,-10,…,-10), (100,100,…,100), (-100,-100,…,-100).
21	Rosenbrock	100, 500, 1000	(2,2,…,2), (5,5,…,5), (10,10,…,10), (25,25,…,25). (2,2,…,2), (5,5,…,5),(10,10,…,10),(-10,-10,…,-10)

22	Whiteholst	100, 500, 1000	(2,2,…,2),(3,3,…,3), (4,4,…,4), (13,13,…,13). (5,5,…,5),(4,4,…,),(13,13,…,13), (-13,-13,…,-13). (10,10,…,10), (4,4,…,), (13,13,…,13), (-13,-13,…,-13
23	Shallow	100, 500, 1000	(3,3,..,3), (5,5,…,5), (11,11,…,11), (25,25,…,25). (-11,-11,..,-11), (25,25,…,25), (-49,-49,…,-49), (5,5,…,5). (-11,-11,..,-11), (25,25,…,25), (49,49,…,49), (11,11,…,11).
24	General Quartic	100, 500, 1000	(2,2,…,2), (-2,-2,…,-2), (4,4,…,4), (-4,-4,…-4). (2,2,…,2), (-2,-2,…,-2), (4,4,…,4), (-8,-8,…-8).
25	Freudenstein & Roth	100, 500, 1000	(3,3,…,3), (-3,-3,…,-3), (5,5,…,5), (-10,-10,…,-10). (-5,-5,…,-5), (-3,-3,…,-3), (14,14,…,14), (-11,-11,…,-11). (2,2,…,2), (5,5,…,5). (3,3,…,3), (-3,-3,…,-3)
26	Himmilblau	100, 500, 1000	(8,8,…,8), (5,5,…,5), (-14,-14,…,-14), (80,80,…,80). (-8,-8,…,-8), (-50,-50,…,-50), (-14,-14,…,-14), (55,55,…,55).

Figure 1 gives graphical representation of number of iterations and Figure 2 presents the graph to show the performance profile in terms of CPU time. In Fig. 1 and Fig. 2, the left side of figure represents the method which is fastest in solving test problems.
The right side represents the test problems that were successfully solved by each method. Clearly that proposed method is the top performer among the others. The proposed method can solve all the problems either based on number of iteration or CPU time without failure.

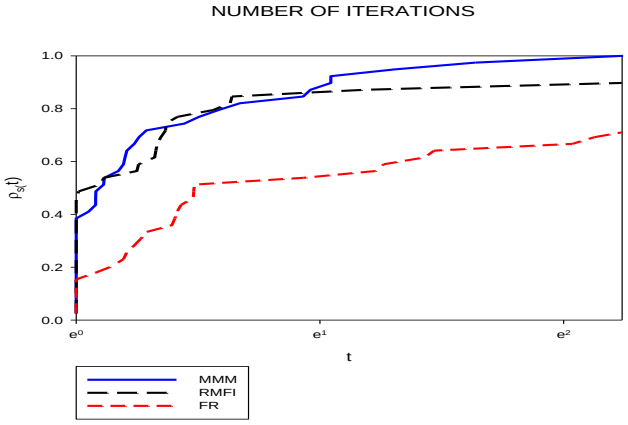


Fig. 1: Performance profile based on the number of iterations.

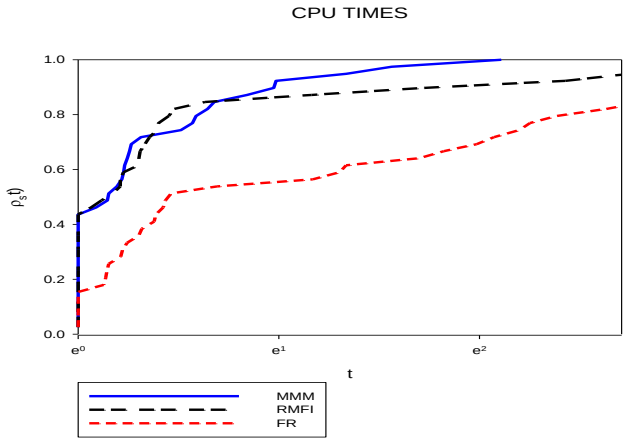


Fig. 2: Performance profile based on CPU time.

5. Conclusion

In this paper, a new proposed named β_k^{MMM} is presented. Based on the result, the method satisfied the sufficiently descent and global convergence properties. Thus, it shows that β_k^{MMM} solves problems with minimum number of iterations and gives the fastest performance in terms of CPU time. The proposed method gives the best performance compared to RMFI [7] and FR [13]. Hence, β_k^{MMM} serves as a good alternative method for solving unconstrained optimization problems.

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