Some Three-Term Conjugate Gradient Algorithms with Descent Condition for Unconstrained Optimization Models

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Abstract: The three-term conjugate gradient methods are among the most efficient numerical methods for solving large-scale unconstrained optimization problems. This is due to their low memory requirements in addition to their global convergence properties. Numerous research and modifications have been done recently to enhanced the performance of this method. This paper presents some modified three-term conjugate gradient methods and show that the methods satisfies the sufficient descent condition. Also, the convergence analysis for general functions was presented under the general Wolfe line search. Preliminary results of some benchmark problems have been reported to illustrates the efficiency of the proposed methods.

Keywords: Three-Term CG method, Sufficient descent, Global convergence, Line search technique, Numerical computations

Introduction

Consider the nonlinear unconstrained optimization problem

$$min\, f(x),\ x \in R^n \qquad (1)$$

where $f(x)$ is continuously differentiable whose gradient $\nabla f(x) = g_x$ is available. Starting with an initial point $x_0 \in R^n$, the conjugate gradient (CG) method computes the sequence of iterates $\{x_k\}$ as follows.

$$x_{k+1} = x_k + \propto_k d_k\ , \quad k = 0,1,2,3,4,\ldots \qquad (2)$$

where $\propto_k > 0$ is the step-length computed along the search direction d_k [19]. For the first iteration d_k is always the Steepest descent direction, that is $d_0 = -g_0$ [18]. However, subsequent directions are recursively computed as.

$$d_k = -g_k + \beta_k d_{k-1},, \quad k \geq 1. \qquad (3)$$

where β_k is the conjugate gradient parameter that characterizes different CG methods. The well-known CG coefficients are Hestenes-Stiefel (HS), Polak-Ribiere-Polyak (PRP), Fletcher-Reeves (FR), Dai-Yuan (DY), Liu-Storey (LS), and Conjugate Descent (CD) [1], [2], with formulas defined as

$$\beta_k^{HS} = \frac{\nabla f_k^T(\nabla f_k - \nabla f_{k-1})}{d_{k-1}^T(\nabla f_k - \nabla f_{k-1})},\ \beta_k^{PRP} = \frac{\nabla f_k^T(\nabla f_k - \nabla f_{k-1})}{\nabla f_{k-1}^T \nabla f_{k-1}},$$

$$\beta_k^{FR} = \frac{\nabla f_k^T \nabla f_k}{\nabla f_{k-1}^T \nabla f_{k-1}},\ \beta_k^{DY} = -\frac{\nabla f_k^T \nabla f_k}{d_{k-1}^T \nabla f_k},$$

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$\beta_k^{LS} = -\frac{\nabla f_k^T(\nabla f_k - \nabla f_{k-1})}{d_{k-1}^T \nabla f_k}, \beta_k^{CD} = -\frac{\nabla f_k^T \nabla f_k}{d_{k-1}^T \nabla f_{k-1}}.$

If α_k is the exact one-dimensional minimizer and $f(x)$ is strictly convex quadratic, then the above CG coefficients would decrease to the linear CG method [1], [2], [4] [22]. Subsequently, if $f(x)$ is non-quadratic, then each choice for β_k would lead to different performance. More so, the method of HS, PRP, and LS performs a restart when the algorithm moves with a small step-size along d_k such that $\nabla f_k - \nabla f_{k-1} \approx 0$. The restart property plays an essential role in the numerical performance of these methods. The global convergence proof of the algorithms of HS, PRP, and LS has been established under various line search procedures [3]. However, for general objective functions, d_k may not be a descent direction. Thus, the convergence proof of these method is yet to be established under the Wolfe-type line search. This has led to several modification of the CG methods that can reduce the evaluation cost of $f(x)$ under the inexact line search.

Recently, Sulaiman et al. [4] presented a new coefficient as follows.

$$\beta_k^{SMARZ} = \frac{g_k^T\left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} d_{k-1}\right)}{d_{k-1}^T(d_{k-1} - g_k)} \tag{4}$$

Motivated by the descent and convergence properties, Sulaiman et al. [5] extended the idea of SMARZ and proposed a variant of (4) named β_k^{SMAR} and defined as

$$\beta_k^{SMAR} = \frac{g_k^T\left(g_k - \frac{\|g_k\|}{\|g_{k-1}\|} d_{k-1}\right)}{\|d_{k-1}\|^2} \tag{5}$$

This method β_k^{SMAR} retained the numerator of SMARZ and inherit some nice properties SMARZ such as the restart property and efficient numerical performance. It is obvious that β_k^{SMARZ} reduces to β_k^{SMAR} if exact minimization rule is applied. Unfortunately, the convergence of these methods was only established under the exact line search.

This paper specifically focusses on three-term CG methods. Beale [6] was among the early researchers that proposed the general three-term CG method. Using the coefficient of β_k^{HS}, he defined a new search direction as

$$d_k = -g_k + \beta_k d_{k-1} + \gamma_k d_t \tag{6}$$

where d_t is the restart directions and $\gamma_k = 0$ for $k = t + 1$, and

$$\gamma_k = \frac{g_k^T y_t}{d_t^T y_t} \quad k > t + 1 \tag{7}$$

The performance of this method was improved using an efficient restart strategy developed by [7] and [8]. The following conditions

$$g_k^T d_k \geq \varphi \|g_k\| \|d_k\|$$

and Powell-Beale condition

$$|g_{k-1}^T g_k| < 0.2\|g_k\|^2$$

are imposed on (6) so that it satisfies the sufficient descent condition. Further research on the three-term conjugate gradient algorithm includes that of [9] who proposed a three term CG method (TTPRP) using the coefficient of β_k^{PRP} as follows.

$$d_k = -g_k + \beta_k d_{k-1} + \gamma_k d_t$$

where $\gamma_k = \frac{g_k^T d_{k-1}}{g_{k-1}^T g_{k-1}}$,and extended the result to β_k^{HS} and named (TTHS) [10] as follows.

$$d_k = \begin{cases} -g_k & if\ s_{k-1}^T y_k < \varepsilon_1 \|g_{k-1}\|^r s_{k-1}^T s_{k-1}, \\ -g_k + \beta_k^{HS} + \gamma_{k-1} \emptyset_{k-1} \text{otherwise} \end{cases}$$

where $\gamma_k = \frac{g_k^T d_{k-1}}{d_{k-1}^T y_{k-1}}$ and $s_{k-1} = x_k - x_{k-1}, r \geq 0, \varepsilon_1 > 0$. An attractive feature of these methods is that

$$\boldsymbol{g_k^T d_k} = -\|\boldsymbol{g_k}\|^2 \tag{8}$$

holds irrespective of the line search procedure employed. The global convergence of TTPRP was established under a modified Armijo line search and that of TTHS under the standard Wolfe line search. For more studies and recent reference on three-term conjugate gradient methods, interested researchers may refer to [3], [9], [11], [12].

In this paper, we extended the methods of SMARZ and SMAR to propose some three-term conjugate gradient methods for unconstrained optimization problems. These proposed methods followed from the structure of TTPRP method and would reduce to the classical SMAR method if exact minimization rule is employed. A review of the literature shows that these methods satisfies the sufficient descent conditions irrespective of the line search procedure.

The rest of the paper is structured as follows. In Sect. 2, we present the algorithms of the proposed methods with some properties. In sect. 3, we give the convergence analysis under some mild conditions. In sect. 4, we report some numerical computations to support the convergence analysis and illustrate the efficiency of the methods. Finally, the conclusions and suggestions for future research are discussed in the last section.

A class of three-term conjugate gradient methods and their algorithms

In an attempt to improve the three-term conjugate gradient method, [3] proposed the three-term TTRMIL and TTMRMIL CG methods based on the structure of TTPRP [9]. In this section, we developed the structure and analysis of TTPRP on the SMARZ and SMAR conjugate gradient methods to achieve (8). The proposed three-term conjugate gradient algorithms are denoted as TTSMAR and TTSMARZ methods and defined as:

$$d_0 = -g_0,\ d_k = -g_k + \beta_k^{SMARZ} d_{k-1} + \gamma_k \emptyset_{k-1} \tag{9}$$

and

$$d_0 = -g_0,\ d_k = -g_k + \beta_k^{SMAR} d_{k-1} + \gamma_k \emptyset_{k-1} \tag{10}$$

where

$$\gamma_k = \frac{g_k^T d_{k-1}}{d_{k-1}^T d_{k-1}} \tag{11}$$

and

$$\emptyset_{k-1} = g_k - \frac{\|g_k\|}{\|g_{k-1}\|} d_{k-1}$$

The algorithms of the of the proposed TTSMARZ and TTSMAR is described as follows.

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Algorithm 2.1. Three-term CG methods of TTSMARZ and TTSMAR

Step 1. Initialization: given $x_0 \epsilon R^n$, $d_0 = -g_0$, set $k := 0$. If $\|g_k\| \leq \varepsilon$,, then stop. Else,
Step 2. Compute β_k by (4) or (5)
Step3. Compute γ_k by (11).
Step 4. Determine the step length $\alpha_k$satisfying (12) and (13)

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta \alpha_k g_k^T d_k, \tag{12}$$

$$g_k^T d_k \geq \sigma g_k^T d_k \tag{13}$$

Step 5. Update the new point based on (2).
Step 6. Check if $\|g_k\| = 0$, then stop. Else, go to step 2 with $k = k + 1$.

The structure of the proposed TTSMARZ and TTSMAR algorithms are similar to the three-term PRP (TTPRP) and other three-term conjugate gradient algorithm. However, we proposed new coefficients β_k and three-term parameter γ_k (see (9), (10), and (11)) which differentiate TTSMARZ and TTSMAR from others methods.

The convergence analysis of TTSMARZ and TTSMAR methods will be discussed in the next section. Before that, we need to show that the directions d_k defined by (9) and (10) satisfies the sufficient descent condition.

Lemma 2.1. Suppose that the $\{d_k\}$ is generated by the algorithm (2.1); where d_k is defined by (9) and (10) and $\gamma_k$is given as (11), then

$$g_k^T d_k \leq -\|g_k\|^2 \quad \forall k \geq 0$$

Proof.From (4), (5), (9), (10), (11), it follows

$$d_k^T g_k = -\|g_k\|^2 + g_k^T d_{k-1}\beta_k - \frac{g_k^T d_{k-1} \cdot g_k^T \emptyset_{k-1}}{d_{k-1}^T d_{k-1}}$$

$$= -\|g_k\|^2 + g_k^T d_{k-1}\beta_k - \frac{g_k^T d_{k-1} \cdot g_k^T \emptyset_{k-1}}{d_{k-1}^T d_{k-1}}$$

$$\leq -\|g_k\|^2$$

This complete the proof. ■

$$g_k^T d_k \leq -\varphi \|g_k\|^2 \quad \forall k \geq 0. \tag{14}$$

This lemma has shown that d_k is a descent direction where $\varphi = 1$

Convergence Analysis

For the convergence analysis of the proposed TTSMARZ and TTSMAR algorithms, we would need the following Assumptions.

Assumption 1. The level set $\Omega = \{x \in R^n / f(x) \leq f(x_0)\}$ is bounded.

Assumption 2. In some neighborhood N of the level set Ω, f is bounded below on R^n and continuously differentiable and its gradient $g(x)$ is Lipchitz continuous in N, such that, there exist a constant $L > 0$ satisfying

$$g_k^T d_k \leq -\varphi \|g_k\|^2 \quad \forall k \geq 0 \tag{15}$$

From assumptions 1 and 2, it implies that there exists a constant $\mu \geq 0$ such that).

$$\|g(x)\| \leq \mu \ \forall x \in \Omega \tag{16}$$

In this analysis, we assume $g_k \neq 0, \ \forall k \geq 0$, otherwise we say a stationary point has been found. Also, we need to coerce the choice of α_k in order to establish the convergence proof. The following lemma, often referred to the Zoutendijk condition, is usually used in the convergence analysis of the CG algorithms. It was originally given by Wolfe [13] and Zoutendijk [15] with the Wolfe line search. This lemma will be use to show that the Zoutendijk condition holds for the proposed TTSMARZ (9) and TTSMAR (10) method under the general Wolfe line search (12) and (13).

Lemma 3.1. Suppose the above Assumptions 1 and 2 holds true. Consider the sequence generated by (2), where α_k satisfies (9), (10), (12), (13) and the direction d_k is descent, then

$$\sum_{k\geq 1} \frac{\left(g_{k-1}^T d_{k-1}\right)^2}{\|d_{k-1}\|^2} < +\infty \tag{17}$$

Lemma 3.2. Suppose assumptions 1 and 2 holds true. Let the sequences $\{g_k\}$ and $\{d_k\}$ be generated by the proposed methods. Then, there exists a positive constant $M > 0$ such that

$$\|d_{k-1}\| \geq M \ \forall k \geq 1. \tag{18}$$

Numerical Results

This section reports the performance of numerical computations of the proposed algorithms compared with the classical SMARZ, SMAR, and TTPRP algorithms under the general Wolfe line search. All unconstrained optimization test problems considered in Table 1 are from Andrei [20]. For each problem function, four initial guesses are used, ranging from points close to the solution to points further from it. All iterations are terminated when $\|g_k\| \leq 10^{-6}$. All algorithms are coded on Matlab version (2015a) and run a Corei5 processor. We employ the performance profiles suggested by [17] to analyze the performance of the proposed methods based on number of iterations and CPU time and compare with the existing methods. The computational performance is shown in Figures 1 and 2, respectively.

The numerical results obtained from the computation are graphed and presented in form of performance profile for easier analysis. Figures 1 and 2 show theperformance of various methods based on number of iterations and CPU time respectively.

Figures 1(a) and 1(b) presented the performance of TTSMARZ compared to the classical SMARZ and TTPRP methods. The result show that TTSMARZ has the best performance in terms of number of iteration and CPU time. Also, Figures 2(a) and 2(b) shows that the proposed TTSMAR outperformed the methods of SMAR and TTPRP.

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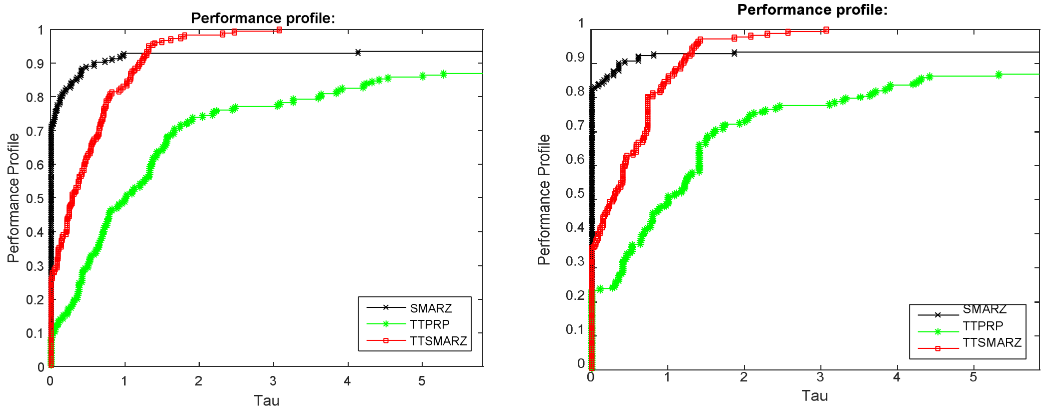
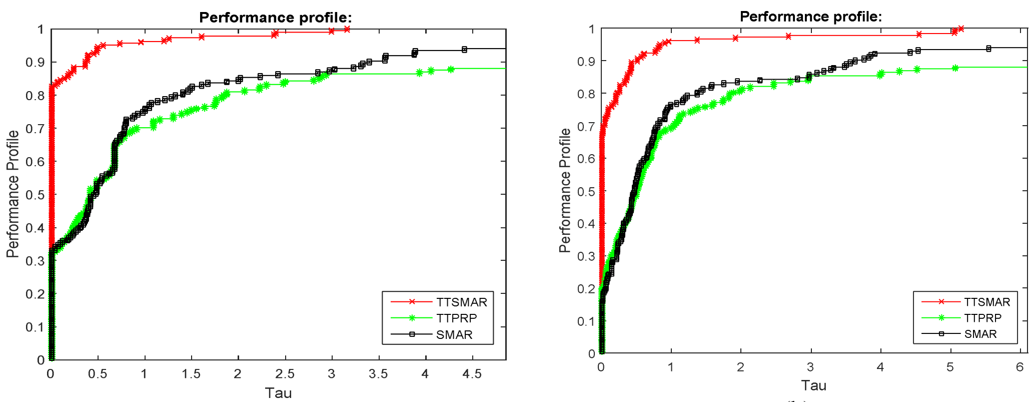
Table 1: List of Test Functions

Function	Dimension	Initial Points
Three Hump Camel	2	(0.5, 0.5), (5, 5), (10, 10), (15, 15)
Booth	2	(2, 2), (9, 9), (10, 10), (13, 13)
Treccani	2	(2, 2), (9, 9), (10, 10), (13, 13)
DQDRTIC	2	(2, 2), (9, 9), (10, 10), (13, 13)
Ext DENCHNB	2	(5,5), (10,10), (20,20), (50,50)
Sphere	2	(2, 2), (9, 9), (10, 10), (15, 15)
Ext Tridiagonal 1	2	(2, 2), (9, 9), (10, 10), (15, 15)
Ext Rosenbrock	2	(0, 0), (2, 2), (10, 10), (15, 15)
Fletcher	2	(2, 2), (3, 3), (9, 9), (10, 10)
Ext White and Holst	2	(0, 0), (2, 2), (10, 10), (13, 13)
Gen Tridiagonal	2	(0, 0), (2, 2), (6, 6), (9, 9)
Diagonal 4	2	(2, 2), (9, 9), (10, 10), (15, 15)
NONSCOMP	2	(2, 2), (9, 9), (10, 10), (15, 15)
Ext Quadratic QP2	2	(2, 2), (9, 9), (10, 10), (15, 15)
Gen Quartic	2	(2, 2), (9, 9), (10, 10), (15, 15)
Ext DENCHNB	4	(5,5,5,5), (10,10,10,10), (20,20,20,20), (50,50,50,50)
Sphere	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
Ext Tridiagonal 1	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
Ext Rosenbrock	4	(0,0,0,0), (2,2,2,2), (10,10,10,10), (15,15,15,15)
Fletcher	4	(2,2,2,2), (3,3,3,3), (9,9,9,9), (10,10,10,10)
Ext White and Holst	4	(0,0,0,0), (2,2,2,2), (10,10,10,10), (13,13,13,13)
Gen Tridiagonal	4	(0,0,0,0), (2,2,2,2), (6,6,6,6), (9,9,9,9)
Diagonal 4	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
NONSCOMP	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
Ext Quadratic QP2	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
Gen Quartic	4	(2,2,2,2), (9,9,9,9), (10,10,10,10), (15,15,15,15)
Sphere	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Tridiagonal 1	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Rosenbrock	100	(0,0, …, 0), (2,2, …, 2), (10,10, …, 10), (15,15, …, 15)
Fletcher	100	(2,2, …, 2), (3,3, …, 3), (9,9, …, 9), (10,10, …, 10)
Ext White and Holst	100	(0,0, …, 0), (2,2, …, 2), (10,10, …, 10), (13,13, …, 13)
Gen Tridiagonal	100	(0,0, …, 0), (2,2, …, 2), (6,6, …, 6), (9,9, …, 9)
Diagonal 4	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
NONSCOMP	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Quadratic QP2	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Gen Quartic	100	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Tridiagonal 1	1000	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Rosenbrock	1000	(0,0, …, 0), (2,2, …, 2), (10,10, …, 10), (15,15, …, 15)
Fletcher	1000	(2,2, …, 2), (3,3, …, 3), (9,9, …, 9), (10,10, …, 10)
Ext White and Holst	1000	(0,0, …, 0), (2,2, …, 2), (10,10, …, 10), (13,13, …, 13)
Gen Tridiagonal	1000	(0,0, …, 0), (2,2, …, 2), (6,6, …, 6), (9,9, …, 9)
Diagonal 4	1000	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
NONSCOMP	1000	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Ext Quadratic QP2	1000	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)
Gen Quartic	1000	(2,2, …, 2), (9,9, …, 9), (10,10, …, 10), (15,15, …, 15)



(a) (b)

Figure 1: Performance Profile of TTSMARZ based on number of iterations (a) and CPU time (b)



(a) (b)

Figure 2: Performance Profile of TTSMAR based on number of iterations (a) and CPU time (b)

Conclusion

The three-term CG algorithms represent a stimulating numerical innovation which give rise to efficient CG methods. Numerous variants of the three-term CG algorithms can be explored using the proposed search directions computed as

$$d_0 = -g_0, \qquad d_k = -g_k + \beta_k d_{k-1} + \gamma_k \emptyset_{k-1}.$$

Several studies and modification of the conjugate gradient methods have been done recently; we suggest to researcher interested in this field to consider some of the efficient CG coefficients β_k and defined a descent direction d_k for unconstrained optimization problem. Also, an application of the CG method can be referred to [21].

In this paper, a class of three-term CG algorithms named TTSMARZ and TTSMAR are proposed based on the efficient conjugate gradient coefficients of SMARZ and SMAR. The idea was based on the structure of the classical TTPRP algorithm. The proposed method satisfies the sufficient descent condition and the convergence analysis was discussed under the general Wolfe line search. Numerical computations using the unconstrained optimization bench mark problems have been presented which shows that the proposed algorithms are efficient and faster than the classical algorithms of TTPRP, SMAR, and SMARZ. This has shown that the proposed methods are easy to implement and thus can be used as alternatives for solving unconstrained optimization problems

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