

A Computational Globally Convergent Spectral CG-Algorithm for solving Unconstrained Nonlinear Problems

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ABSTRACT

In this paper, we are concerned with the Conjugate Gradient (CG) methods for solving unconstrained nonlinear optimization problems. It is well-known that the direction generated by a CG-method may not be a descent direction for the objective function. In this paper, we have done a little modification to the Conjugate Descent (CD) method such that the direction generated by the modified method provides a descent direction for any objective function. This property depends neither on the line search used, nor on the convexity of the objective function. Moreover, the modified method reduces to the standard CD-method if line search is exact. Under mild conditions, we have proved that the modified method with strong Wolfe line search is globally convergent even if the objective function is non convex. We have also presented some numerical tests to show the efficiency of the new proposed algorithm.

Keywords. Spectral Conjugate Gradient, Global Convergence, Unconstrained Optimization, Descent Direction, Line Search.

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1. INTRODUCTION

Our aim in this paper is to study the stability and global convergence properties for a new proposed algorithm and to do some practical computational tests to show the performance of the new nonlinear spectral CG-method which are suitable for unconstrained optimization problems with the well-known Powell restarting criterion (Powell, 1977) and with appropriate mid conditions. Now, we consider the following unconstrained optimization problem:

$$\min \{f(x) | x \in R^n\} \quad (1)$$

where, $f: R^n \rightarrow R$ is a continuously differentiable function. Nonlinear CG-algorithms are efficient for solving (1). These algorithms are generating iterates by letting:

$$x_{k+1} = x_k + \alpha_k d_k, \quad k = 0, 1, \dots \quad (2)$$

with

$$d_k = \begin{cases} -g_k, & \text{if } k = 0 \\ -g_k + \beta_k d_{k-1}, & \text{if } k \geq 1 \end{cases} \quad (3)$$

where, x_k is the current iteration, $\alpha_k > 0$ is the step-length which is determined by Wolfe line search method, d_k is the new search direction, $g_k = g(x_k)$ denotes the gradient of f at x_k , and β_k is a suitable parameter. There are many well-known formulas for β_k , such as:

$$\begin{aligned} \text{Fletcher-Reeves (FR)} \quad & \left(\beta_k^{FR} = \frac{g_k^T g_k}{g_{k-1}^T g_{k-1}} \right) \quad (\text{Fletcher and Reeves, 1964}) \\ \text{Polak Ribière (PR)} \quad & \left(\beta_k^{PR} = \frac{y_{k-1}^T g_k}{g_{k-1}^T g_{k-1}} \right) \quad (\text{Polak and Ribière, 1969}) \quad (4) \\ \text{Conjugate-Descent (CD)} \quad & \left(\beta_k^{CD} = \frac{g_k^T g_k}{-d_{k-1}^T g_{k-1}} \right) \quad (\text{Fletcher, 1987}) \end{aligned}$$

The CG-algorithm is a powerful line search method for solving optimization problems, and it remains very popular for engineers and mathematicians who are interested in solving large-scale complicated test problems. This method can avoid, the computation and storage of some matrices associated with the Hessian of objective functions. where $\|\cdot\|$ denotes the Euclidean norm of vectors. An important property of the CD-method is that it will produce a descent direction under the strong Wolfe line search. In the strong Wolfe line search, the step-length α_k is required to satisfy the following (Wolfe, 1969):

$$\begin{aligned} f(x_k + \alpha_k d_k) &\leq f(x_k) + \delta \alpha_k g_k^T d_k \\ |g(x_k + \alpha_k d_k)^T d_k| &\leq -\sigma g_k^T d_k \\ 0 &< \delta < \sigma < 1. \end{aligned} \quad (5)$$

Another popular CG-algorithm to solving problem (1) is the Spectral CG-algorithm (SCG) method, which was developed originally by (Barzilai and Borwein, 1988). The main feature of this method is that only gradient directions are used at each line search whereas a non-monotone strategy guarantees the global convergence property. As well as, this method outperforms the sophisticated CG-algorithm in many complicate test problems. The direction d_k of the spectral CG-algorithm is given by the following way:

$$d_k = -\theta_k g_k + \beta_k d_{k-1} \quad (6)$$

where the parameter β_k is computed by:

$$\beta_k = \frac{(\theta_k y_{k-1} - s_{k-1})^T g_k}{s_{k-1}^T y_{k-1}} \quad (7)$$

and, θ_k is taken to be the spectral gradient and computed by the following:

$$\theta_k = \frac{s_{k-1}^T s_{k-1}}{s_{k-1}^T y_{k-1}} \quad (8)$$

where, $y_{k-1} = g_k - g_{k-1}$, $s_{k-1} = x_k - x_{k-1}$. The numerical results in some practices show that these type of methods are very effective. Unfortunately, they cannot guarantee to generate descent directions.

Recently, Spectral CG-algorithm have also been reported in (Liu; et al , 2012); (Liu and Jiang, 2012); (ILivieris and Pintelas, 2013) and (Liu; Zhang and Xu, 2014) .

However, (Liu; et al , 2012) take a modification to the standard CD-method such that the direction generated in their method (say, LDW) is always a descent direction and d_k is defined by the following:

$$d_k^{LDW} = \begin{cases} -g_k, & \text{if } k = 1 \\ -\theta_k^{LDW} g_k + \beta_k d_{k-1}, & \text{if } k \geq 2 \end{cases} \quad (9)$$

where, β_k is specified by the following relation:

$$\beta_k = \begin{cases} \beta_k^{CD}, & \text{if } g_k^T d_{k-1} \leq 0, \\ 0, & \text{else,} \end{cases} \quad (10)$$

and

$$\theta_k^{LDW} = 1 - \frac{g_k^T d_{k-1}}{g_{k-1}^T d_{k-1}}; \quad \beta_k = \beta^{CD} + \min(0, \frac{-g_k^T d_{k-1}}{y_{k-1}^T d_{k-1}} \beta^{CD}) \quad (11)$$

Recently, (Al-Bayati and Al-Khayat, 2013) have developed another spectral CG-algorithm (say, KH) for solving unconstrained optimization problems. They have done a little modification to the standard CD-method such that the search direction generated by their modified method provides a descent direction for the objective function. They also present some numerical results to show the efficiency of their proposed method. Namely, their search directions are similar to the search direction given by Liu et al (9):

$$d_k^{KH} = \begin{cases} -g_k, & \text{if } k = 1 \\ -\theta_k^{KH} g_k + \beta_k^{CD} d_{k-1}, & \text{if } k \geq 2 \end{cases} \quad (12)$$

with a an efficient new value for the spectral θ_k^{KH} defined by:

$$\theta_k^{KH} = -\frac{d_{k-1}^T y_{k-1}}{d_{k-1}^T g_{k-1}} - \frac{d_{k-1}^T g_k g_k^T g_{k-1}}{\|g_k\|^2 d_{k-1}^T g_{k-1}} \quad (13)$$

They prove that their method can guarantee to generate descent directions with globally convergent rate of convergence.

2. A NEW SPECTRAL CG-METHOD.

In this section we have, first, to investigate how to determine a descent direction of any general objective function. Let x_k be the current iterate and let d_k be defined by:

$$d_k^{New} = \begin{cases} -g_k, & \text{if } k = 0 \\ -\theta_k^{New} g_k + \beta_k^{CD} d_{k-1}, & \text{if } k \geq 1 \end{cases} \quad (14)$$

where, β_k^{CD} is specified by (1.4) with the following new parameter:

$$\theta_k^{New} = 1 - \left(\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \right) \left(\frac{d_{k-1}^T g_k}{\|g_k\|^2} \right) - \frac{d_{k-1}^T g_k}{2g_{k-1}^T g_{k-1}} \quad (15)$$

This new proposed spectral CG-method reduces to the standard CD-method if the line search is exact. But generally we refer to use the inexact line search (Wolfe line search). We have first to prove that d_k is a sufficiently descent direction.

2.1 LEMMA

Suppose that d_k^{New} is defined by (14) and (15). Furthermore, assume that the parameter α_k satisfies strong Wolfe condition (5) with $\sigma_k < 0.5$. Then, the following result:

$$g_k^T d_k \leq -c_1 \|g_k\|^2 \quad (16)$$

holds for any $k \geq 0$.

PROOF.

$$\text{If } k = 0, \text{ then } d_0^T g_0 = -\|g_0\|^2 \quad (17)$$

We suppose that the condition (16) is true for all values of $k-1$; i.e.

$$d_{k-1}^T g_{k-1} = -\|g_{k-1}\|^2 \quad (18)$$

Then, by induction we have to prove that the condition (16) is true for all values of k , i.e.

$$g_k^T d_k = -\theta_k^{New} \|g_k\|^2 + \beta_k^{CD} g_k^T d_{k-1} \quad (19)$$

From (4); (14), and (15), it follows that:

$$g_k^T d_k = - \left[1 - \left(\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \right) \left(\frac{d_{k-1}^T g_k}{\|g_k\|^2} \right) - \frac{d_{k-1}^T g_k}{2g_{k-1}^T g_{k-1}} \right] \|g_k\|^2 - \frac{\|g_k\|^2}{d_{k-1}^T g_{k-1}} g_k^T d_{k-1} \quad (20)$$

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

$$g_k^T d_k = - \left[1 - \frac{d_{k-1}^T g_k}{d_{k-1}^T g_{k-1}} - \frac{d_{k-1}^T g_k}{2g_{k-1}^T g_{k-1}} + \frac{g_k^T d_{k-1}}{d_{k-1}^T g_{k-1}} \right] \|g_k\|^2$$

$$g_k^T d_k = - \left[1 - \frac{d_{k-1}^T g_k}{2g_{k-1}^T g_{k-1}} \right] \|g_k\|^2 \quad (21)$$

From second Wolfe condition defined in (5), we have:

$$d_{k-1}^T g_k \leq -\sigma d_{k-1}^T g_{k-1}; \sigma \text{ive} \quad (22)$$

Therefore (21) becomes:

$$g_k^T d_k \leq - \left[1 + \frac{\sigma d_{k-1}^T g_{k-1}}{2g_{k-1}^T g_{k-1}} \right] \|g_k\|^2 \quad (23)$$

From (18) we have:

$$g_k^T d_k \leq - \left[1 + \frac{\sigma g_{k-1}^T g_{k-1}}{2g_{k-1}^T g_{k-1}} \right] \|g_k\|^2 \quad (24)$$

Hence:

$$g_k^T d_k \leq - \left[1 + \frac{\sigma}{2} \right] \|g_k\|^2 \quad (25)$$

Implies:

$$g_k^T d_k \leq -c \|g_k\|^2 \quad \text{with} \quad c = [1 + \sigma/2] > 0 \quad (26)$$

Thus, we obtain the desired result.

From **Lemma 2.1**, it is known that d_k is a descent direction of f at x_k . Furthermore, if an exact line search is used, then:

$$\theta_k^{New} = 1 - \left(\frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \right) \left(\frac{d_{k-1}^T g_k}{\|g_k\|^2} \right) - \frac{d_{k-1}^T g_k}{2g_{k-1}^T g_{k-1}} = 1 \quad (27)$$

In this case, the new proposed spectral CD-method reduces to the standard CD-method. However, it is often that the exact line search is time-consuming and sometimes is unnecessary. In the following, we are going to develop a new spectral CG-algorithm, where the search direction d_k is chosen by (14)-(15) and the step-length is determined by strong Wolfe-type inexact line search.

2.2 AN ACCELERATED LINE SEARCH PARAMETER.

In this section we take advantage of this behavior of CG-algorithms and consider an acceleration scheme which was presented in (Andrei, 2009). In accelerated algorithm instead of (2) the new estimation of the minimum point is computed as:

$$x_{k+1} = x_k + \lambda_k \alpha_k d_k \quad (28)$$

where

$$\lambda_k = -\frac{a_k}{b_k} \quad (29)$$

$$a_k = \alpha_k g_k^T d_k, b_k = -\alpha_k (g_k - g_z)^T d_k, g_z = \nabla f(z) \text{ and } z = x_k + \alpha_k d_k$$

Hence, the new estimation of the solution is computed as in (28). Therefore, using the above acceleration scheme (28) and (29) we can present the following new spectral CG-algorithm.

2.3 Outline of the New Algorithm (NEW):

Step 1: Initialization: Take $x_0 \in R^n$; set the parameters $0 < \delta \leq \sigma < 1$.

Compute $f(x_0)$ and $g_0 = \nabla f(x_0)$, set $d_0 = -g_0$ for $k = 0$.

Step 2: Line Search: Compute $\alpha_k > 0$ satisfying the Wolfe line search

condition and compute $z = x_k + \alpha_k d_k$, $y_k = g_k - g_z$, $g_z = \nabla f(z)$.

Acceleration scheme: compute, $a_k = \alpha_k g_k^T d_k$, $b_k = -\alpha_k y_k^T d_k$, If

$b_k \neq 0$, then compute, $\lambda_k = -\frac{a_k}{b_k}$ and update the variables as

$x_{k+1} = x_k + \lambda_k \alpha_k d_k$, otherwise update the variables as

$x_{k+1} = x_k + \alpha_k d_k$.

Step 3: Test for Convergence: If $\|g_k\|_\infty \leq \text{eps}$ is satisfied then the iterations are stopped, eps. is small positive number.

Step 4: Restarting Criterion: If Powell restarting criterion s. t.

$$|g_k^T g_{k-1}| \geq 0.2 \|g_k\|^2 \quad (30)$$

is satisfied then do a restart step by SD-direction; otherwise continue.

Step 5: Computation of New Scalar Parameters:

$$\left(\beta_k^{CD} = \frac{g_k^T g_k}{-d_{k-1}^T g_{k-1}} \right)$$

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

Step 6: New Search Direction: Compute the new Spectral search direction

$$d_k = -\theta_k^{New} g_k + \beta_k^{CD} d_{k-1}$$

Step 7: New Iteration: Set $k=k+1$ and go to Step 2.

It is well known that, if f is bounded along the direction d_k , then there exists a step length α_k satisfying the Wolfe line search conditions (5). In our new proposed spectral CG-algorithm, when the Powell restarting condition (30) is satisfied, then we restart the algorithm with the negative gradient. Under reasonable assumptions, conditions (5) and (30) are sufficient to prove the global convergence of the new proposed algorithm.

3. CONVERGENCE ANALYSIS.

In this section, we are in a position to study the global convergence property of the new proposed spectral CG-algorithm defined in (15). We first state the following mild assumptions, which will be used in the proof of global convergence property.

Assumption (H):

- (i) The level set $S = \{x : x \in R^n, f(x) \leq f(x_1)\}$ is bounded, where x_1 is the starting point.
- (ii) In a neighborhood Ω of S , f is continuously differentiable and its gradient g is Lipschitz continuously, namely, there exists a constant $L \geq 0$ such that

$$\|g(x) - g(x_k)\| \leq L \|x - x_k\|, \forall x, x_k \in \Omega \quad (31)$$

Obviously, from the Assumption (H, i) there exists a positive constant D such that:

$$D = \max\{\|x - x_k\|, \forall x, x_k \in S\} \quad (32)$$

where D is the diameter of Ω . From Assumption (H, ii), we also know that there exists a constant $\Gamma \geq 0$, such that:

$$\|g(x)\| \leq \Gamma, \forall x \in S \quad (33)$$

On some studies of the CG-methods, the sufficient descent or descent condition plays an important role. Unfortunately, this condition is hard to hold.

3.1 A New Theorem

Under Assumptions (H, i) and (H, ii), suppose that d_k is given by (14) and (15) where α_k satisfies strong Wolfe condition (5) with $\sigma_k < 0.5$ then it holds that

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0 \quad (34)$$

Proof.

Suppose that there exists a positive constant $\varphi > 0$ such that:

$$\|g_k\| \geq \varphi \quad (35)$$

For all k . Then, from (14), it follows that:

$$\begin{aligned} \|d_k\|^2 &= d_k^T d_k \\ &= (-\theta_k^{New} g_k + \beta_k^{CD} d_{k-1})(-\theta_k^{New} g_k + \beta_k^{CD} d_{k-1}) \\ &= (\theta_k^{New})^2 \|g_k\|^2 - 2\theta_k^{New} \beta_k^{CD} d_{k-1}^T g_k + (\beta_k^{CD})^2 \|d_{k-1}\|^2 \end{aligned}$$

Since $d_k = -\theta_k^{New} g_k + \beta_k^{CD} d_{k-1}$ then:

$$\begin{aligned} &= (\theta_k^{New})^2 \|g_k\|^2 - 2\theta_k^{New} (d_k^T + \theta_k^{New} g_k^T) g_k + (\beta_k^{CD})^2 \|d_{k-1}\|^2 \\ &= (\theta_k^{New})^2 \|g_k\|^2 - 2\theta_k^{New} g_k^T d_k - 2(\theta_k^{New})^2 \|g_k\|^2 + (\beta_k^{CD})^2 \|d_{k-1}\|^2 \\ &= (\theta_k^{New})^2 \|d_{k-1}\|^2 - 2\theta_k^{New} g_k^T d_k - (\theta_k^{New})^2 \|g_k\|^2 \end{aligned} \quad (36)$$

Divide both sides of the above equality by $(g_k^T d_k)^2$, then from (4), (16), (31) and (36) we obtain:

$$\frac{\|d_k\|^2}{(g_k^T d_k)^2} = \frac{(\beta_k^{CD})^2 \|d_{k-1}\|^2 - 2\theta_k^{New} g_k^T d_k - (\theta_k^{New})^2 \|g_k\|^2}{(g_k^T d_k)^2} \quad (37)$$

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

From (26)

$$g_k^T d_k \leq -c \|g_k\|^2$$

$$\leq \left[\frac{\|g_k\|^2}{c \|g_{k-1}\|^2} \right]^2 \frac{\|d_{k-1}\|^2}{c^2 \|g_k\|^4} - (\theta_k^{New})^2 \frac{\|g_k\|^2}{c^2 \|g_k\|^4} - 2\theta_k^{New} \frac{1}{c \|g_k\|^2} \quad (38)$$

Reformulate; add and subtract a positive number yields:

$$\leq \frac{\|d_{k-1}\|^2}{c^4 \|g_{k-1}\|^4} - \left\{ (\theta_k^{New} \frac{\|g_k\|}{c \|g_k\|^2})^2 + 2\theta_k^{New} \frac{1}{c \|g_k\|^2} \right\} + \frac{1}{\|g\|^2} - \frac{1}{\|g\|^2} \quad (39)$$

$$\leq \frac{\|d_{k-1}\|^2}{c^4 \|g_{k-1}\|^4} - \left\{ (\theta_k^{New} \frac{\|g_k\|}{c \|g_k\|^2})^2 + 2\theta_k^{New} \frac{1}{c \|g_k\|^2} + \frac{1}{\|g\|^2} \right\} + \frac{1}{\|g\|^2}$$

$$\leq \frac{\|d_{k-1}\|^2}{c^4 \|g_{k-1}\|^4} - \left[\theta_k^{New} \frac{\|g_k\|}{c \|g_k\|^2} + \frac{1}{\|g_k\|} \right]^2 + \frac{1}{\|g_k\|^2} \quad (40)$$

$$\leq \frac{\|d_{k-1}\|^2}{c^4 \|g_{k-1}\|^4} + \frac{1}{\|g_k\|^2} \text{ mid term of (40) is always positive followed by negative sign}$$

From (31) and since:

$$\|d_1\|^2 = -d_1^T g_1 = \|g_1\|^2 \quad (41)$$

We get:

$$\frac{\|d_k\|^2}{(d_k^T g_k)^2} \leq \sum_{i=1}^k \frac{1}{\|g_i\|^2} \quad (42)$$

Therefore, from (42) and (35) we have:

$$\frac{(d_k^T g_k)^2}{\|d_k\|^2} \geq \frac{\varphi}{k} \quad (43)$$

which indicates:

$$\sum_{k=1}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} \Rightarrow +\infty \quad (44)$$

Which makes a contradiction to our assumption (34). Hence the proof of this theorem is complete.

4. NUMERICAL EXPERIMENTS

The main work of this section is to report the performance of the new proposed spectral CG-method **NEW** on a set of fifty five complicated test problems. The original codes were written by (Andrei, 2008) in FORTRAN language and in double precision arithmetic and modified in this research paper to make it suitable to evaluate all algorithms considered in this paper. All the tests were performed on a PC. Our experiments were performed on the selected set of nonlinear unconstrained problems that have second derivatives available. These test problems are contributed in CUTE (Bongartz et al, 1995) and their details are given in the Appendix. for each test function we have considered four different numerical experiments with number of variables $n = 100, 400, 700$ and 1000 and we have concerned only on the total of all of these dimensions for all tools used in these comparisons. All these methods terminate when the following stopping criterion is met.

$$\|g_k\|_{\infty} \leq 10^{-5} \quad (45)$$

we also force these routines stopped if the iterations (NOI) exceed 1000 or the number of function evaluations (NOF) reach 2000 without achieving the minimum. In all these tables(n) indicates as a dimension of the problem; (NOI) number of iterations; (NOF) number of function evaluations.

In **Table (4.1)** we assess the reliability of the standard **CD**-method, against the standard **FR**; **PR** classical CG-methods using standard Wolfe conditions as a line search subroutine and using the same group of our test problems.

In **Table (4.2)** we have compared the percentage performance of the standard **CD**-method against **FR** and **PR** CG-methods, using the standard Wolfe conditions as a line search subroutine. Now, taking over all the tools as 100% , in order to summarize our numerical results, we have concerned only on the total of four different dimensions $n = 100, 400, 700, 1000$, for all tools used in these comparisons.

In **Tables (4.3)** we assess the reliability of our new proposed spectral CG-algorithm, **NEW** against some recent spectral CG-algorithms like **LDW**; **KH** spectral CG-methods using both standard and modified Wolfe conditions as a line search subroutine respectively and using the same set of test problems.

In **Table (4.4)** we have compared the percentage performance of the new proposed spectral CG-algorithm **NEW** against **KH** and **LDW**, spectral CG algorithms using both standard and modified Wolfe conditions as a line search subroutine respectively. Now, taking over all the tools as 100%, in order to summarize our numerical results, we have concerned only on the total of four different dimensions $n = 100, 400, 700, 1000$, for all tools used in these comparisons.

Table (4.1a): Comparisons between FR; PR & CD Algorithms

No. of Test Functions	FR		PR		CD	
	NOI	NOF	NOI	NOF	NOI	NOF
1	235	389	268	470	265	426
2	23	52	23	52	23	52
3	47	126	54	129	47	126
4	53	148	53	148	53	148
5	72	151	80	163	72	149
6	17	46	17	46	17	46
7	26	61	24	59	25	60
8	29	71	30	73	29	71
9	20	55	20	55	20	55
10	22	58	22	58	22	58
11	22	50	17	40	22	50
12	163	329	164	331	163	329
13	26	95	38	115	26	95
14	7	25	7	25	7	25
15	30	90	30	90	30	90
16	29	59	29	59	29	59
17	33	73	33	74	33	72

18	29	78	30	79	29	78
19	18	33	18	33	18	33
20	4	12	4	12	4	12
21	1438	2320	1575	2122	1699	2556
22	25	69	25	69	25	69
23	69	200	105	230	68	194
24	4	12	4	12	4	12
25	7	16	7	16	7	16
26	4	8	4	8	4	8
27	34	59	37	63	34	59
28	19	65	19	65	19	65
29	23	54	23	54	23	54
30	31	52	31	52	31	52

Table (4.1b) Comparisons between FR; PR & CD Algorithms

No. of Test Functions	FR		PR		CD	
	NOI	NOF	NOI	NOF	NOI	NOF
31	25	54	25	54	25	54
32	24	48	22	41	24	48
33	58	135	58	129	58	135
34	73	151	81	173	75	154
35	23	59	23	59	23	59
36	17	46	17	46	17	46
37	24	36	24	36	24	36
38	23	62	23	62	23	62
39	30	60	31	61	30	60
40	59	138	58	140	55	132
41	19	55	19	55	19	55
42	41	95	47	111	41	95
43	20	44	20	44	20	44
44	57	134	59	141	57	134
45	10	35	10	35	10	35
46	13	43	13	43	13	43
47	7	27	7	27	7	27
48	16	72	16	72	16	72
49	33	73	33	74	33	72
50	24	64	24	64	24	64
51	117	250	118	236	120	266
52	4	12	4	12	4	12
53	77	154	74	154	76	153
54	8	16	8	16	8	16
55	21	60	21	60	21	60
TOTAL	3382	6779	3626	6747	3671	7053

Table (4.2) Percentage Performance of CD against FR and PR

Tools	CD	FR	PR
NOI	100%	92%	98%
NOF	100%	96%	95%

Clearly, this table shows that the CD-method is the worse, because it does not generate sufficiently descent search directions in general. For this reason many Authors deal with improving the search direction of this method by implementing spectral CG-methods (as we will show in the next table). From this table we can conclude that both FR and PR are very close to each other, while CD needs some an additional necessary conditions to become an effective method. Numerical results of this table indicates that FR saves about (8)% NOI and (4)% NOF to complete solving this set of selected complicated nonlinear test problems, while PR saves about (2)% NOI and (5)% NOF to complete solving this set of selected complicated nonlinear test problems.

Table (4.3a) Comparisons between KH; LDW & NEW Spectral Algorithms

No. of Test Functions	KH		LDW		NEW	
	NOI	NOF	NOI	NOF	NOI	NOF
1	154	332	122	331	48	56
2	23	52	23	52	24	72
3	55	148	59	148	39	79
4	53	148	53	148	26	103
5	69	135	67	132	69	77
6	17	46	17	46	14	25
7	22	53	22	53	24	82
8	29	71	29	71	32	62
9	20	55	20	55	18	51
10	22	58	22	58	9	20
11	24	51	24	51	15	24
12	166	333	164	329	72	101
13	27	105	35	113	8	20
14	7	25	7	25	7	22
15	30	90	30	90	29	77
16	29	59	29	59	27	83
17	34	76	36	78	20	52
18	26	72	26	72	24	83
19	18	33	18	33	14	38
20	4	12	4	12	8	16
21	1113	2017	1158	2058	85	132
22	24	67	24	67	27	45
23	59	173	76	205	22	39

24	4	12	4	12	5	19
25	7	16	7	16	7	17
26	4	8	4	8	16	47
27	27	52	27	46	42	93
28	19	65	19	65	14	45
29	23	54	23	54	16	26
30	31	52	31	52	22	33

Table (4.3b): Comparisons between KH; LDW& NEW Spectral Algorithms

No. of Test Functions	KH		LDW		NEW	
	NOI	NOF	NOI	NOF	NOI	NOF
31	25	54	25	54	23	34
32	23	46	24	48	25	36
33	56	124	55	123	35	46
34	78	167	79	164	62	96
35	23	59	23	59	18	53
36	17	46	17	46	14	25
37	28	44	28	44	28	40
38	23	62	23	62	30	62
39	29	57	29	57	23	58
40	60	138	58	134	27	92
41	19	55	19	55	16	26
42	44	98	43	99	36	62
43	20	44	20	44	8	20
44	62	142	64	149	34	45
45	10	35	10	35	18	26
46	13	43	13	43	11	44
47	7	27	7	27	11	19
48	16	72	16	72	10	22
49	34	76	36	78	22	48
50	24	65	24	65	22	41
51	95	219	99	222	74	170
52	4	12	4	12	4	16
53	73	146	76	158	75	120
54	8	16	8	16	8	20
55	21	60	21	60	15	27
Total	2952	6377	3001	6465	1432	2887

Table (4.4) Percentage Performance of NEW against KH and LDW

Tools	LDW	KH	NEW
NOI	100%	98%	47%
NOF	100%	98%	44%

Numerical results of this table indicates that NEW spectral CG-algorithm saves about (53)% NOI and (56)% NOF compared with the spectral CG-algorithm LDW-method and about (51)% NOI and (54)% NOF against spectral KH-algorithm to complete solving the set of selected complicated nonlinear test problems.

CONCLUSIONS

There exists a large variety of CG-algorithms. In this paper, we have presented a new spectral CG-algorithm in which the parameter g_k is computed as $\theta_k g_k$. For uniformly convex functions, if the step-size d_k approaches zero, the gradient is bounded and the line search satisfies the strong Wolfe conditions, then our new spectral CG-algorithm is globally convergent. For general nonlinear functions, if the parameter θ_k is bounded, then our new spectral CG-algorithm is globally convergent.

The performance percentage of our new proposed algorithm is very effective compared with other established CG-algorithms for the selected set of test problems found in the CUTE library. However, in general among the six CG algorithms mentioned in this paper, we have found that the CD algorithm is the worse and the new proposed spectral CG algorithm is the best. The arrange of these algorithms as shown in this paper is given by:

CD (the worse)-----PR-----FR-----LDW-----KH-----NEW (the best).

6. APPENDIX

The details of all selected test problems can be found in CUTE (Bongartz et al, 1995):

- 1) Extended Freudenstein & Roth
- 2) Extended Trigonometric Function
- 3) Extended Beale Function
- 4) Extended Penalty Function
- 5) Raydan 1 Function
- 6) Raydan 2 Function
- 7) Diagonal2 Function
- 8) Hager Function
- 9) Generalized Tridiagonal-1 Function
- 10) Extended Tridiagonal-1 Function
- 11) Extended Three Exponential Terms
- 12) Generalized Tridiagonal-2
- 13) Diagonal4 Function
- 14) Diagonal5 Function
- 15) Extended Himmelblau Function
- 16) Generalized PSC1 Function
- 17) Extended PSC1 Function
- 18) Extended Block Diagonal BD1 Function
- 19) Extended Cliff CLIFF
- 20) Quadratic Diagonal Perturbed Function
- 21) Extended Wood Function

- 22) Extended Quadratic Penalty QP1 Function
- 23) Extended Quadratic Penalty QP2 Function
- 24) Extended EP1 Function
- 25) Extended Tridiagonal-2 Function
- 26) ARWHEAD
- 27) NONDQUAR
- 28) EG2
- 29) DIXMAANA
- 30) DIXMAANB
- 31) DIXMAANC
- 32) DIXMAANE
- 33) Partial Perturbed Quadratic
- 34) Broyden Tridiagonal
- 35) EDENSCH Function
- 36) DIAGONAL 6
- 37) DIXON3DQ
- 38) ENGVAL1
- 39) DENSCHNA
- 40) DENSCHNC
- 41) DENSCHNB
- 42) DENSCHNF
- 43) BIGGSB1
- 44) Extended Block-Diagonal BD2
- 45) Generalized quartic GQ1 function
- 46) Diagonal 7
- 47) Diagonal 8
- 48) Full Hessian
- 49) SIN COS
- 50) Generalized quartic GQ2 function
- 51) EXTROSNB
- 52) ARGLINB
- 53) FLETCHCR
- 54) HIMMELBG
- 55) HIMMELBH

REFERENCES

- [1]. M.J.D. Powell, (1977), "Restart Procedures for the Conjugate Gradient Method". Mathematical Program. 12, 241–254.
- [2]. R. Fletcher and C. M. Reeves, (1964), "Function Minimization by Conjugate Gradients" The Computer Journal. 7, 149–154.
- [3]. E. Polak and G. Ribière, (1969), "Note Sur la Convergence de Methods de Directions Conjugates". 3(16), 35–43.
- [4]. R. Fletcher, (1987), Practical Methods of Optimization: Unconstrained Optimization. John Wiley & Sons, New York, NY, USA.
- [5]. P. Wolfe, (1969), "Convergence Conditions for Ascent Methods". SIAM Rev. 11, 226–235J.
- [6]. Barzilai and J. M. Borwein, (1988), "Two-Point Step Size Gradient Methods". IMA Journal of Numerical Analysis. 8(1), 141–148.
- [7]. J. Liu; X. Du, and K. Wang, (2012), "A Mixed Spectral CD-DY Conjugate Gradient Method". Hindawi Publishing Corporation, Journal of Applied Mathematics. Article ID 569795.
- [8]. J. Liu and Y. Jiang, (2012), "Global Convergence of a Spectral Conjugate Gradient Method for Unconstrained Optimization". Hindawi Publishing Corporation, Article ID 758287.
- [9]. I. E. Livieris and P. Pintelas (2013) A new class of spectral conjugate gradient methods based on a modified secant equation for unconstrained optimization Journal of Computational and Applied Mathematics 239, 396–405.
- [10]. D. Liu; L. Zhang and G. Xu (2014) Spectral method and its application to the conjugate gradient method Applied Mathematics and Computation 240 (2014) 339–347.
- [11]. Al-Bayati, A.Y. and Al-Khayat, H. N. (2013) A Global Convergent Spectral Conjugate Gradient Method) Australian Journal of Basic and Applied Sciences, 7(7): 302-309.
- [12]. N. Andrei, , (2009) Acceleration of conjugate gradient algorithms for unconstrained optimization, Applied Mathematical Computational, 213, 361–369.
- [13]. N. Andrei, (2008), '40 Conjugate Gradient Algorithms for Unconstrained Optimization, a Survey on their Definition'. ICI Technical Report. No. 13/08, March 14.
- [14]. K. E. Bongartz; A.R. Conn, N.I.M. Gould and P.L. Toint, (1995), "CUTE: Constrained and Unconstrained Testing Environments". ACM Trans, Math. Software. 21, 123-160.