

A New Conjugate Gradient Algorithm for Minimization Problems Based on the Modified Conjugacy Condition

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Abstract Optimization refers to the process of finding the best possible solution to a problem within a given set of constraints. It involves maximizing or minimizing a specific objective function while adhering to specific constraints. Optimization is used in various fields, including mathematics, engineering, economics, computer science, and data science, among others. The objective function can be a simple equation, a complex algorithm, or a mathematical model that describes a system or process. There are various optimization techniques available, including linear programming, nonlinear programming, genetic algorithms, simulated annealing, and particle swarm optimization, among others. These techniques use different algorithms to search for the optimal solution to a problem. In this paper, the main goal of unconstrained optimization is to minimize an objective function that uses real variables and has no value restrictions. In this study, based on the modified conjugacy condition, we offer a new conjugate gradient (CG) approach for nonlinear unconstrained problems in optimization. The new method satisfied the descent condition and the sufficient descent condition. We compare the numerical results of the new method with the Hestenes-Stiefel (HS) method. Our novel method is quite effective according to the number of iterations (NOI) and the number of functions (NOF) evaluated, as demonstrated by the numerical results on certain well-known non-linear test functions.

Keywords Optimization Problems, Conjugate Gradient Algorithm, Descent Condition, Global Convergence

1. Introduction

Suppose the optimization problem as an example

$$\text{Min } f(x), x \in R^n \quad (1.1)$$

where $f: R^n \rightarrow R$ is a continuously differentiable, real-valued function. Starting from a first guess $x_1 \in R^n$, a nonlinear conjugate gradient algorithm creates the sequence $\{x_k\}$, defined as

$$x_{k+1} = x_k + \alpha_k d_k \quad (1.2)$$

Or $x_{k+1} = x_k + v_k$ where $v_k = \alpha_k d_k = x_{k+1} - x_k$

Here, a line search is used to determine the step size α_k , and the search direction is denoted by d_k . The steepest descent direction, $d_1 = -g_1$, is often the search direction in the first iteration. The other search directions are follows:

$$d_{k+1} = -g_{k+1} + \beta_k d_k \quad (1.3)$$

where g_k is a gradient of f at x_k and β_k is a parameter known as a conjugate parameter. Different conjugate gradient methods have been developed as a result of the literature presenting several choices for β_k . Some classic conjugate parameters are Fletcher-Reeves (FR) method [1], the Hestenes-Stiefel (HS) method [2], and the Polak-Ribière (PR) method [3], Dai and Yuan (DY) [4], which are respectively determined as follows:

$$\beta_k^{FR} = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \quad (1.4)$$

$$\beta_k^{HS} = \frac{g_{k+1}^T y_k}{d_k^T y_k} \tag{1.5}$$

$$\beta_k^{PR} = \frac{g_{k+1}^T y_k}{g_k^T g_k} \tag{1.6}$$

$$\beta_k^{DY} = \frac{\|g_{k+1}\|^2}{d_k^T (g_{k+1} - g_k)} \tag{1.7}$$

Where $y_k = g_{k+1} - g_k$. The Euclidean norm of vectors is represented by the letter $\|\cdot\|$. Global convergence properties of conjugate gradient methods are those that have received the most attention. Several writers, including Gilbert and Nocedal [5] and Hestenes and Stiefel [2], have investigated the convergence of conjugate gradient algorithms under various line searches. Several studies have also been conducted to enhance the conjugate gradient method's parameters, including ([6] and [7]):

$$\beta_k = \frac{g_{k+1}^T g_{k+1}}{d_k^T y_k} - \mu \left(\frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \right)^2 \tag{1.8}$$

$$\beta_k = \mu \frac{\|g_{k+1}\|^2}{-d_k^T g_k} \left(1 + \left(k \frac{d_k^T g_{k+1}}{\|y_k\|^2} \right) \left(\frac{\|g_{k+1}\|^2}{d_k^T g_k} \right) \right), \tag{1.9}$$

The structure of this essay is as follows: We'll introduce a novel conjugate gradient method suggestion in Section 2. In section 3, we present proof of the descent and sufficient descent conditions of the new method. Many numerical tests of a new conjugate gradient technique are presented in Section 4. Our last remarks are presented in Section 5.

2. Derivation the New Method

In this part, we will derive our new method. Consider the vector below

$$\bar{g}_{k+1} = g_{k+1} + (1 - \delta) \left(\frac{g_{k+1}}{\gamma} \right) - \mu g_{k+1} \tag{2.1}$$

where, $\delta \in (0,1)$, $\mu = 0.1$ and $\gamma = \frac{2\sqrt{\omega}}{\|v_k\|} (1 + \|x_{k+1}\|)$

and ω is the machine error. Now, suppose that the modified conjugacy condition is

$$d_{k+1}^T y_k = -\bar{g}_{k+1}^T v_k \tag{2.2}$$

and the search direction is given by

$$d_{k+1} = -g_{k+1} + \beta_k^{new} d_k \tag{2.3}$$

multiply both sides by y_k , to get

$$d_{k+1} y_k = -g_{k+1} y_k + \beta_k^{new} d_k y_k \tag{2.4}$$

then,

$$-\bar{g}_{k+1}^T v_k = -g_{k+1} y_k + \beta_k^{new} d_k y_k \tag{2.5}$$

here, we get

$$\beta_k^{new} = \frac{g_{k+1} y_k - \bar{g}_{k+1} v_k}{d_k^T y_k} \tag{2.6}$$

3. Algorithm of A New C. G. Method

1. select x_1 and $\varepsilon = 10^{-5}$.
2. set $d_1 = -g_1$, $g_k = \nabla f(x_k)$, set $k = 1$
3. compute the step length $\alpha_k > 0$ satisfying the Wolf line search $f(x_k + \alpha_k d_k) - f(x_k) \leq c_1 \alpha_k g_k^T d_k$

$$|g_{k+1}^T d_k| \leq c_2 |g_k^T d_k|, \text{ where, } 0 < c_1 < c_2 < 1.$$

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

$$g_{k+1} = \nabla f(x_{k+1}), \text{ If } \|g_{k+1}\| \leq \varepsilon,$$

then stop.

5. Calculate β_k^{new} by

$$\beta_k^{new} = \frac{g_{k+1}^T y_k - \bar{g}_{k+1}^T v_k}{d_k^T y_k}$$

6. Compute $d_{k+1} = -g_{k+1} + \beta_k^{new} d_k$
7. If $|g_{k+1}^T g_k| > 0.2 \|g_{k+1}\|^2$ then return to step 2.

Else

Set $k = k + 1$ and return to step 3.

4. The Descent and Sufficient Descent Property of the New Method

Theorem 1: The direction in (1.3) with the new CG (2.6) satisfies the descent requirement, i.e. $d_{k+1}^T g_{k+1} \leq 0$, with both an exact and an inexact line searches, if the sequence $\{x_k\}$ is created by (1.2).

Proof: The equation $d_{k+1} = -g_{k+1} + \left(\frac{g_{k+1} y_k - \bar{g}_{k+1} v_k}{d_k^T y_k} \right) d_k$

Implies that

$$d_{k+1} = -g_{k+1} + \left(\frac{g_{k+1} y_k}{d_k^T y_k} - \frac{\bar{g}_{k+1} v_k}{d_k^T y_k} \right) d_k \tag{3.1}$$

Multiplying the above equations from the right sides by g_{k+1} , we obtain

$$d_{k+1}^T g_{k+1} = -\|g_{k+1}\|^2 + \frac{g_{k+1} y_k}{d_k^T y_k} d_k^T g_{k+1} - \frac{\bar{g}_{k+1} v_k}{d_k^T y_k} d_k^T g_{k+1} \tag{3.2}$$

If an exact line search is used to determine the step size which is $d_k^T g_{k+1} = 0$, then we get $d_{k+1}^T g_{k+1} \leq 0$.

If we have an inexact line search which is $d_k^T g_{k+1} \neq 0$. Using mathematical induction, from the first search direction, we get $d_1^T g_1 = -\|g_1\|^2 \leq 0$. We assume that it is true for case k , that is mean $d_k^T g_k \leq 0$. To prove case $k + 1$.

Because the HS parameter satisfies the descent requirement, the first two terms of the above equation are less than or equal to zero. To complete the proof, we only need proof that the third term is

$$-\frac{\bar{g}_{k+1}^T v_k}{d_k^T y_k} d_k^T g_{k+1} = -\left(\frac{v_k^T (g_{k+1} + (1-\delta)\left(\frac{g_{k+1}}{\gamma}\right) - \mu g_{k+1})}{d_k^T y_k}\right) d_k^T g_{k+1}$$

Since, $\delta \in (0,1)$, $\mu = 0.1$ and $\gamma = \frac{2\sqrt{\omega}}{\|v_k\|}(1 + \|x_{k+1}\|)$

$$0 < \|v_k\| = \|x_{k+1} - x_k\| \leq \|x_{k+1}\| \Rightarrow 0 \leq \frac{\|v_k\|}{2\sqrt{\omega} + \|x_{k+1}\|} \leq 1$$

So, we get

$$-\frac{\bar{g}_{k+1}^T v_k}{d_k^T y_k} d_k^T g_{k+1} = -\left(1 + \left(\frac{(1-\delta)}{\gamma}\right) - (1-\delta)\mu\right) \frac{\alpha_k (d_k^T g_{k+1})^2}{d_k^T y_k} < 0$$

Finally, we have $d_{k+1}^T g_{k+1} \leq 0$.

Theorem 2: suppose that $\{x_k\}$ is generated by (1.2), then the direction in (1.3) with the new CG (2.2) satisfies the sufficient descent requirement, i.e. $d_{k+1}^T g_{k+1} \leq -C \|g_{k+1}\|^2$.

Proof: Consider the equation

$$d_{k+1} = -g_{k+1} + \left(\frac{g_{k+1}^T y_k - \bar{g}_{k+1}^T v_k}{d_k^T y_k}\right) d_k \quad (3.3)$$

Implies that

$$d_{k+1} = -g_{k+1} + \left(\frac{g_{k+1}^T y_k}{d_k^T y_k} - \frac{\bar{g}_{k+1}^T v_k}{d_k^T y_k}\right) d_k \quad (3.4)$$

By multiplying both sides of above equation by g_{k+1} from right, we obtain

$$d_{k+1}^T g_{k+1} = -\|g_{k+1}\|^2 + \frac{g_{k+1}^T y_k}{d_k^T y_k} d_k^T g_{k+1} - \frac{\bar{g}_{k+1}^T v_k}{d_k^T y_k} d_k^T g_{k+1} \quad (3.5)$$

Since the parameter of HS is to satisfy the descent property, then we get the following inequality

$$\begin{aligned} d_{k+1}^T g_{k+1} &\leq -\frac{\bar{g}_{k+1}^T v_k}{d_k^T y_k} d_k^T g_{k+1} \\ &= -\left(\frac{v_k^T (g_{k+1} + (1-\delta)\left(\frac{g_{k+1}}{\gamma}\right) - \mu g_{k+1})}{d_k^T y_k}\right) d_k^T g_{k+1} \\ &\leq -\left(1 + \left(\frac{(1-\delta)}{\gamma}\right) - (1-\delta)\mu\right) \frac{\alpha_k (d_k^T g_{k+1})^2}{d_k^T y_k} * \frac{\|g_{k+1}\|^2}{\|g_{k+1}\|^2} \end{aligned} \quad (3.6)$$

Let $C = \left(1 + \left(\frac{(1-\delta)}{\gamma}\right) - (1-\delta)\mu\right) \frac{\alpha_k (d_k^T g_{k+1})^2}{d_k^T y_k} * \frac{1}{\|g_{k+1}\|^2}$

Then, we have $d_{k+1}^T g_{k+1} \leq -C \|g_{k+1}\|^2$.

Now, to show the global convergence of our new conjugate gradient method, the following presumptions are necessary [8].

Assumption 1. The level set $S = \{x: x \in R^n, f(x) \leq f(x_0)\}$ is bounded. i.e. $\exists B > 0$ such that

$$\|x\| \leq B, \quad \forall x \in S \quad (3.7)$$

Assumption 2. In a neighborhood $\Omega \in S$, E is differentiable and its gradient g is Lipschitz continuous, i.e. $\exists L > 0$ such that

$$\|g(w) - g(w_k)\| \leq L \|w - w_k\|, \quad \forall w, w_k \in \Omega \quad (3.8)$$

From Assumptions 1 and 2, $\exists M > 0$ such that

$$\|g(w)\| \leq M, \quad \forall w \in S. \quad (3.9)$$

Lemma 1 [9]. Suppose that the above Assumptions true and the $\{x_k\}$ is a sequence constructed by equations (1.2) and (1.3), where d_k satisfies the descent property and the step size is computed by strong Wolfe conditions. If

$$\sum_{k \geq 1} \frac{1}{\|d_k\|^2} = \infty \quad (3.10)$$

Then

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0. \tag{3.11}$$

Theorem 3. Assume that the above Assumptions hold. If the iteration is computed from equations (1.2) and (1.3) where β_k^{new} is defined in (2.6), and α_k satisfies the strong Wolfe line search conditions, then

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0$$

Proof: From equations (1.3) and (2.6), we have

$$\begin{aligned} \|d_{k+1}\| &\leq \|g_{k+1}\| + \left| \frac{g_{k+1}^T y_k - g_{k+1}^T v_k}{d_k^T y_k} \right| \|d_k\|, \\ \|d_{k+1}\| &\leq \|g_{k+1}\| + \left(\left| \frac{g_{k+1}^T y_k}{d_k^T y_k} \right| + \left(1 + \frac{(1-\delta)}{\gamma} - \mu\right) \left| \frac{g_{k+1}^T v_k}{d_k^T y_k} \right| \right) \|d_k\| \\ \|d_{k+1}\| &\leq \|g_{k+1}\| + \left(\left| \frac{g_{k+1}^T y_k}{d_k^T y_k} \right| + \left(1 + \frac{(1-\delta)}{\gamma} - \mu\right) \left| \frac{g_{k+1}^T v_k}{d_k^T y_k} \right| \right) \|d_k\| \end{aligned} \tag{3.12}$$

Since $g_{k+1}^T v_k \leq \alpha_k d_k^T y_k$ and by using (3.9), also from Lipschitz Condition $\|y_k\| \leq L\|v_k\|$ and $g_{k+1}^T y_k \leq Lg_{k+1}^T d_k$ where $L > 0$, we have

$$\|d_{k+1}\| \leq M + \left(L + \left(\left(1 + \frac{(1-\delta)}{\gamma} - \mu\right) \alpha_k \right) \right) \|d_k\| \tag{3.13}$$

since, $\|v_k\| = \|x - x_k\|$, and $D = \max\{\|x - x_k\|, \forall x, x_k \in R\}$.

It follows that

$$\|d_{k+1}\| \leq M + \left(L + \left(\left(1 + \frac{(1-\delta)}{\gamma} - \mu\right) \alpha_k \right) \right) D \alpha_k = \beta$$

this implies that $\sum_{k \geq 1} \frac{1}{\|d_{k+1}\|^2} \geq \sum_{k \geq 1} \frac{1}{\beta^2} = \infty$

and so, $\sum_{k \geq 1} \frac{1}{\|d_{k+1}\|^2} = \infty$

By using lemma (1), we get $\liminf_{k \rightarrow \infty} \|g_k\| = 0$, which completes the proof.

5. Numerical Results

This section is designed to evaluate how effectively the new CG method has been used. We conduct a number of computational experiments on a concatenation of test problems for unconstrained nonlinear optimization derived from [10]. To demonstrate the application and efficacy of the suggested approach with various dimensions of $4 \leq n \leq 5000$, all programs are written in the FORTRAN95 language. The performance of the new CG method and the original CG method using NOI and NOF for 7 different non-linear functions is compared in Table 1. Table 2 shows that the rate of improvement for the modified CG technique illustrates how it outperforms the standard method in terms of NOI and NOF.

Table 1. Comparison Between Two Algorithms (HS. and New CG)

Test function.	DIM.	HS		New.	
		NOI	NOF	NOI	NOF
G-Cantrel	4	22	159	18	113
	10	22	159	18	113
	100	22	159	19	129
	500	23	171	21	144
	1000	23	171	21	144
	5000	28	248	32	255
G-Wolfe	4	11	24	11	25
	10	32	65	31	63
	100	49	99	48	101
	500	52	105	57	127
	1000	70	141	57	119
	5000	165	348	62	139
Powell	4	37	102	34	95
	10	37	102	34	95
	100	40	117	34	95
	500	44	136	34	95
	1000	44	136	34	95
	5000	44	136	37	112
Rosen	4	30	83	30	83
	10	30	83	30	83
	100	30	83	30	83
	500	30	83	30	83
	1000	30	83	30	83
	5000	30	83	30	83
Miele	4	28	85	28	84
	10	31	102	28	84
	100	33	114	34	118
	500	40	146	35	120
	1000	46	176	41	152
	5000	54	211	48	188
G-Wood	4	30	68	26	61
	10	30	68	26	61
	100	30	68	26	61
	500	30	68	26	61
	1000	30	68	27	63
	5000	30	68	27	63
OSP.	4	8	45	8	49
	10	13	58	12	46
	100	49	185	51	194
	500	112	353	107	327
	1000	156	475	156	473
	5000	256	774	256	774
Total		1951	6208	1744	5536

Table 2. The Percentage of Improving of New Algorithm

Tools	HS	New CG
NOI	100%	89.3906 %
NOF	100%	89.1753 %

The suggested strategy raises NOI and NOF by 10.6094% and 10.8247%, respectively. The modified New CG method has generally outperformed the standard HS approach by a factor of 10.71705%.

6. Conclusions

For unconstrained optimization issues, we proposed a new conjugate gradient algorithm in this paper. The decent condition and sufficient decent condition, which are essential steps of the proofs with an exact line search and an inexact line search. Based on the numerical results, it can be clearly observed that the new algorithm is more efficient in terms of the number of iteration and the number of function evaluation.

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