Using a new type of formula conjugate on the gradient methods

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| Article Info | ABSTRACT | | | | |
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| Article history: | Unconstrained optimization problems, such as energy minimization, can be | | | | |
| Received Apr 7, 2022 Revised May 10, 2022 Accepted Jun 2, 2022 | solved using the conjugate gradient method. For its major characteristic, the optimal formula conjugate encompasses all conjugate gradient algorithms. In conjugate gradient approaches, the formula conjugate is typically the focus point and it's playing a very important role for conjugate gradient approaches. To offer the essential descent criteria in this work, we devised a | | | | |
| Keywords: | novel formula based on the second order Taylor which have the descent property too. Our research focused on our suggested method's-convergence | | | | |
| Conjugate gradient Convergence property Descent property Formula conjugate gradient | property with Wolfe condition is established and numerical performance. Comparison to FR-method, the new algorithem shows significant improvement in numerical results. | | | | |
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Numerical results

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1. INTRODUCTION

The main goal of this study is to present an efficient optimization approach for minimizing a function's objective function $f: \mathbb{R}^n \to \mathbb{R}$, see [1]. The following equation gives the usual form of iterations for discovering the extreme points of the function:

$$x_{k+1} = x_k + \alpha_k \mathbf{d}_k \tag{1}$$

certainly, α_k and d_k are the most significant aspects of an optimization model (1), and they determine the effectiveness of a technique. Hassan [2] has further information. The length of a step can be determined by:

$$\alpha_k = -\frac{d_k^T d_k}{d_k^T Q d_k} \tag{2}$$

typically, the Wolfe line search criteria [3], [4] are used to determine the step length α_k in (1):

$$f(x_k + \alpha_k \mathbf{d}_k) \le f(x_k) + \delta \alpha_k \mathbf{g}_k^T \mathbf{d}_k$$
(3)

$$\mathbf{d}_k^T \mathbf{g}(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \ge \sigma \mathbf{d}_k^T \mathbf{g}_k \tag{4}$$

where $0 < \delta < \sigma < 1$. The vector direction is computed as follows in the general conjugate gradient method:

$$\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k \tag{5}$$

notice that (4) is a generic update formula for the conjugate gradient parameter-based search direction computation. The key point in various literatures (refer to [5]-[8]) is to pick the scalar β_k , which leads to a variety of conjugate gradient techniques depending on the β_k . Dai *et al.* [1] and Fletcher and Reeves [9] devised the conjugate gradient approach, which goes like this:

$$\beta_k^{FR} = \frac{\|g_{k+1}\|^2}{g_k^T g_k} \quad , \quad \beta_k^{DR} = \frac{\|g_{k+1}\|^2}{g_k^T y_k} \tag{6}$$

denote y_k to be the gradient change. Many conjugate gradient methods have been created, and numerous publications have been written on the subject, addressing both computational and theoretical aspects. Iiduka and Narushima [10], β_k is calculated as:

$$\beta_k^{HY} = \frac{\|g_{k+1}\|^2}{2/\alpha_k (f_k - f_{k+1})} \tag{7}$$

as a result, the parameter's value has changed β_k in [2] is as (8).

$$\beta_k^B = \frac{\|g_{k+1}\|^2}{(f_k - f_{k+1})/\alpha_k - g_k^T d_k/2}$$
(8)

accelerated gradient descent techniques were classified as a subclass of gradient descent methods during the creation of gradient models [11]. Scalar β_k may be chosen in a variety of ways, and a good choice leads to improved convergence. These are descent-direction approaches as well.

In this study, we describe a conjugate gradient technique based on the conjugacy criterion. Our recommended strategy ensures enough descent using any line search. We can establish global convergence of our suggested approach under correct conditions if the line search fits the Wolfe criteria. The numbers suggest that the technique we propose is feasible.

2. DERIVING NEW COEFFICIENT CONJUGATE

The conjugacy condition is well recognized to play a crucial role in convergence analysis and numerical computation. The conjugacy requirement is used in this new strategy. The conjugate gradient approach is such that the conjugacy requirement holds in the situation when f is quadratic model and V is determined using the precise line search, namely:

$$d_{k+1}^{q'}Qd_k = 0 (9)$$

as a result of adding (5) to the previous equation:

$$\beta_k = \frac{\mathsf{d}_{k+1}^T \mathcal{Q}_{s_k}}{\mathsf{d}_k^T \mathcal{Q}_{s_k}} \tag{10}$$

the new conjugate gradient formula is derived using the second order Taylor formula. Allow me to explain:

$$f(x) = f(x_{k+1}) + g_{k+1}^T (x - x_{k+1}) + \frac{1}{2} (x - x_{k+1})^T Q(x_{k+1}) (x - x_{k+1})$$
(11)

the f(x) has the following gradient as:

$$\mathbf{g}_{k+1} = \mathbf{g}_k + Q(x_{k+1})\mathbf{s}_k \tag{12}$$

using (3) with exact line search in (11), we get:

$$s_k^T Q(x_{k+1}) s_k = (f_{k+1} - f_k) + 3/2 \,\alpha_k \mathsf{g}_k^T \mathsf{g}_k \tag{13}$$

To write (13), we have (14).

$$d_k^T Q(x_{k+1}) s_k = (f_{k+1} - f_k) / \alpha_k + 3/2 \, \mathsf{g}_k^T \mathsf{g}_k \tag{14}$$

putting (15) in (10), we obtain:

$$\beta_k = \frac{g_{k+1}^T y_k}{(f_{k+1} - f_k)/\alpha_k + 3/2 g_k^T g_k} \tag{15}$$

we obtain the following results when we use exact line search.

$$\beta_k = \frac{\|g_{k+1}\|^2}{(f_{k+1} - f_k)/\alpha_k + 3/2g_k^T g_k}$$
(16)

As a result of our novel formula, the so-called new method. Using this way, we will obtain the new algorithm which generates different formulae by using the second order Taylor formula and conjugacy condition. However, we may now present a new algorithm as follows, employing our suggested new parameter (16) as:

Step 1: Let $x_1 \in \mathbb{R}^n$ and $d_1 = -d_1$. Put k = 1. **Step 2:** If $||d_{k+1}|| \le 10^{-6}$, then stop.

Step 3: Estimate α_k and which of the three fulfill (3-4) and variables should be updated $x_{k+1} = x_k + \alpha_k d_k$. **Step 4:** Calculate the value of β_k , as defined in (16).

Step 5: Put k = k + 1 and go to 5.

Theorem (2.2): for the new approach, we have the following in the form of (1) and (5), with the new parameter given by (16).

$$d_{k+1}^T g_{k+1} < 0 \text{ and } d_{k+1}^T g_{k+1} = \beta_k d_k^T g_k$$
(17)

Proof: from evident that $d_1 = -g_1$ satisfies $d_1^T g_1 < 0$. Let that $d_k^T g_k < 0$ hold for any k. Straight from (5) and (16) we obtained that:

$$\mathbf{d}_{k+1}^{T}\mathbf{g}_{k+1} = -\mathbf{g}_{k+1}^{T}\mathbf{g}_{k+1} + \beta_{k}\mathbf{d}_{k}^{T}\mathbf{g}_{k+1} = -\beta_{k}((f_{k+1} - f_{k})/\alpha_{k} + 3/2\,\mathbf{g}_{k}^{T}\mathbf{g}_{k})) + \beta_{k}\mathbf{d}_{k}^{T}\mathbf{g}_{k+1}$$
(18)

using (12) in above equation, we get:

$$\mathbf{d}_{k+1}^T \mathbf{g}_{k+1} = \beta_k \mathbf{d}_k^T \mathbf{g}_k \tag{19}$$

since $d_k^T g_k < 0$, then we get:

$$\mathbf{d}_{k+1}^T \mathbf{g}_{k+1} < 0 \tag{20}$$

so the proof is completed.

3. CONVERGENCE ANALYSIS

Each method in the numerical optimization methods has different convergence properties and needed some assumptions. Our recommended strategy ensured enough descent using any line search. In the study of innovative conjugate gradient procedure' global convergence, the assumptions listed below are commonly utilized. Assumption A:

- The bounded level set $\Omega = \{u/f(u) \le f(u_0)\}$.
- The function f is smooth and its gradient is Lipschitz continuous in some neighborhood Ω of L_0 , i.e., where L > 0 constant, such that:

$$\|\mathbf{g}(\mathbf{v}) - \mathbf{g}(\mathbf{z})\| \le \mathbf{L} \|\mathbf{v} - \mathbf{z}\|, \forall \mathbf{v}, \mathbf{z} \in \Omega$$

$$\tag{21}$$

for more details see [12]. In order to prove the convergence property of our new algorithm and some algorithem in optimization, we use the proof idea of a researcher Zoutendijk. The Zoutendijk condition is a lemma that is widely used to check the conjugate gradient technique's global convergence. Zoutendijk was the first to say it in [13].

Lemma (3.1): assume that Assumption A is true. The sequence $\{x_k\}$ produced by any iteration algorithm thus satisfies:

$$\sum_{k=1}^{\infty} \frac{(d_k^T d_k)^2}{\|d_k\|^2} < \infty$$
(22)

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Theorem (3.2): the sequence $\{x_k\}$ created by the new approach meets the following conditions:

$$\lim_{k \to \infty} \inf \left\| \mathsf{g}_k \right\| = 0 \tag{23}$$

Proof: assume that (23) is false by induction. The (8) is changed to $d_{k+1} + d_{k+1} = \beta_k d_k$, and when both sides are squared, we get:

$$\|\mathbf{d}_{k+1}\|^2 + \|\mathbf{g}_{k+1}\|^2 + 2\mathbf{d}_{k+1}^T \mathbf{g}_{k+1} = (\beta_k)^2 \|\mathbf{d}_k\|^2$$
(24)

putting (24), results in:

$$\|\mathbf{d}_{k+1}\|^{2} = \frac{\left(\mathbf{d}_{k+1}^{T}\mathbf{g}_{k+1}\right)^{2}}{\left(\mathbf{d}_{k}^{T}\mathbf{g}_{k}\right)^{2}} \|\mathbf{d}_{k}\|^{2} - 2\mathbf{d}_{k+1}^{T}\mathbf{g}_{k+1} - \left\|\mathbf{g}_{k+1}\right\|^{2}$$
(25)

taking (25) and dividing it by $(\mathbf{d}_{k+1}^T \mathbf{f}_{k+1})^2$, we have:

$$\frac{\|\mathbf{d}_{k+1}\|^2}{(\mathbf{d}_{k+1}^T \mathbf{g}_{k+1})^2} = \frac{\|\mathbf{d}_k\|^2}{(\mathbf{d}_k^T \mathbf{g}_k)^2} = \frac{\|\mathbf{g}_{k+1}\|^2}{(\mathbf{d}_{k+1}^T \mathbf{g}_{k+1})^2} - \frac{2}{\mathbf{d}_{k+1}^T \mathbf{g}_{k+1}}$$
(26)

we may deduce the following from the equation:

$$\frac{\|\mathbf{d}_{k+1}\|^2}{(\mathbf{d}_{k+1}^T\mathbf{g}_{k+1})^2} \le \frac{\|\mathbf{d}_k\|^2}{\left(\mathbf{d}_k^T\mathbf{g}_k\right)^2} - \left(\frac{\|\mathbf{g}_{k+1}\|}{\left(\mathbf{d}_{k+1}^T\mathbf{g}_{k+1}\right)^2} + \frac{1}{\|\mathbf{g}_{k+1}\|^2}\right) + \frac{1}{\|\mathbf{g}_{k+1}\|} \le \frac{\|\mathbf{d}_k\|^2}{\left(\mathbf{d}_k^T\mathbf{g}_k\right)^2} + \frac{1}{\|\mathbf{g}_{k+1}\|^2} \tag{27}$$

Hence,

$$\frac{\|\mathbf{d}_{k+1}\|^2}{(\mathbf{d}_{k+1}^T \mathbf{g}_{k+1})^2} \le \sum_{i=1}^{k+1} \frac{1}{\|\mathbf{g}_i\|^2} \tag{28}$$

let there exists $c_1 > 0$ such that $\|g_k\| \ge c_1$ for all $k \in n$, then:

$$\frac{\|\mathbf{d}_{k+1}\|^2}{(\mathbf{d}_{k+1}^T\mathbf{g}_{k+1})^2} \le \frac{k+1}{c_1^2}$$
(29)

using the assumption and (29) as a guide, we can see that:

$$\sum_{k=1}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} = \infty$$
(30)

we know that $\lim_{k\to\infty} \inf \|g_k\| = 0$ holds because of Lemma 1.

4. NUMERICAL RESULTS

The results of numerical experiments are presented in this section. The FR-Algorithm was compared to the new conjugate gradient algorithm. In Fortran, both algorithms are written. Andrei [14] is where you'll find the test problems. The following papers and references are available to interested readers (Ref. [15]-[19]). We chose (15) unconstrained optimization problems in extended, and we investigated numerical experiments with the amount of variables n=100;1,000 for each test function. As a termination condition, we apply the inequality $\|\underline{g}_{(k+1)}\| \le [10]^{\wedge}(-6)$. Many papers have proposed this method for optimization problems also [20]-[26]. The Wolfe condition test results were collected and reported in Table 1, where each column has the following meanings; δ =0.0001 and σ =0.5. The problem's name is problem, the problem's size is dim, the number of iterations (NOI), and the number of function evaluations are all terms used to describe the problem (NOF). In terms of iterations and function evaluations, Table 1 indicates how many difficulties these methods have resolved.

Table 1 compares the new methods to the Fletcher and Reeves [1] convex optimization technique; as demonstrated in Table 2. The new algorithm saves NI, NR, and NF overall when compared to the conventional Fletcher and Reeves (FR) methodology. Particularly for our collection of test issues, which showed the performance improvement of the new algorithm.

| P. No | n | FR algorithm | | | New .algorithm | | |
|---------------------------|------|--------------|------|------|----------------|-----|------|
| | | NI | ŇR | NF | NI | NR | NF |
| Trigonometric | 100 | 19 | 12 | 35 | 18 | 11 | 33 |
| - | 1000 | 38 | 23 | 65 | 37 | 23 | 65 |
| Extended Rosenbrock | 100 | 47 | 18 | 93 | 40 | 23 | 88 |
| | 1000 | 78 | 45 | 131 | 38 | 21 | 83 |
| Extended Beale | 100 | 32 | 15 | 52 | 16 | 9 | 30 |
| | 1000 | 22 | 10 | 42 | 13 | 7 | 25 |
| Generelized Tridiegonal 1 | 100 | 25 | 11 | 43 | 23 | 8 | 44 |
| | 1000 | 46 | 28 | 741 | 40 | 23 | 528 |
| Extended Tridiagonal 1 | 100 | 32 | 13 | 64 | 16 | 7 | 33 |
| | 1000 | 77 | 46 | 169 | 15 | 6 | 30 |
| Generalized Tridiagonal 2 | 100 | 37 | 8 | 67 | 40 | 15 | 59 |
| | 1000 | 73 | 27 | 115 | 49 | 19 | 77 |
| Extended Himmelblau | 100 | 12 | 5 | 25 | 10 | 6 | 19 |
| | 1000 | 14 | 6 | 29 | 10 | 6 | 19 |
| Extended PSC1 | 100 | 15 | 9 | 31 | 8 | 6 | 17 |
| | 1000 | 8 | 6 | 17 | 7 | 5 | 15 |
| Q. Diagonal Perturbed | 100 | 124 | 41 | 231 | 48 | 9 | 87 |
| | 1000 | 445 | 196 | 711 | 197 | 46 | 352 |
| Extended Wood | 100 | 71 | 35 | 110 | 26 | 11 | 50 |
| | 1000 | 47 | 15 | 84 | 34 | 12 | 65 |
| Extended Hiebart | 100 | 101 | 40 | 217 | 83 | 47 | 190 |
| | 1000 | 101 | 40 | 214 | 86 | 49 | 194 |
| ARWHEAD (CUTE) | 100 | 9 | 4 | 18 | 8 | 5 | 16 |
| | 1000 | 12 | 7 | 82 | 8 | 5 | 16 |
| NONDIA (CUTE) | 100 | 13 | 7 | 25 | 11 | 6 | 22 |
| | 1000 | 15 | 7 | 29 | 9 | 6 | 19 |
| DIXMAANE (CUTE) | 100 | 121 | 65 | 218 | 89 | 34 | 143 |
| | 1000 | 345 | 169 | 634 | 252 | 86 | 400 |
| Partial Perturbed Q | 100 | 74 | 21 | 123 | 79 | 20 | 120 |
| | 1000 | 370 | 88 | 616 | 251 | 66 | 436 |
| Total | | 2423 | 1017 | 5031 | 1561 | 597 | 3275 |

| Table 1. The FR and new methods numerical res | ults |
|---|------|
|---|------|

Table 2. The performance percentage for the new CG algorithm compared with FR method

| | NF | NR | NI |
|------------|--------|--------|--------|
| FR method | 100% | 100% | 100% |
| New method | 64.42% | 58.70% | 65.09% |

CONCLUSION 5.

In this study, we offer a novel nonlinear CG-algorithm based on the strictly convex quadratic function described by (10) that is globally convergent, functional, and fulfills the descent property under certain assumptions. The novel types presented in this research are successful, according to computer studies. The new algorithm was sufficient and effective.

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