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A new conjugate gradient algorithms using conjugacy condition for solving unconstrained optimization

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ABSTRACT

The primarily objective of this paper which is indicated in the field of conjugate gradient algorithms for unconstrained optimization problems and algorithms is to show the advantage of the new proposed algorithm in comparison with the standard method which is denoted as. Hestenes Stiefel method, as we know the coefficient conjugate parameter is very crucial for this reason, we proposed a simple modification of the coefficient conjugate gradient which is used to derived the new formula for the conjugate gradient update parameter described in this paper. Our new modification is based on the conjugacy situation for nonlinear conjugate gradient methods which is given by the conjugacy condition for nonlinear conjugate gradient methods and added a nonnegative parameter to suggest the new extension of the method. Under mild Wolfe conditions, the global convergence theorem and lemmas are also defined and proved. The proposed method's efficiency is programming and demonstrated by the numerical instances, which were very encouraging.

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1. INTRODUCTION

The conjugate gradient method is a group of very important smooth function minimization methods, which is have a large dimension. We are interesting with conjugate gradient method for locating the function's local minimum,

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

where $f: R^n \rightarrow R^1$ is a nonlinear, smooth function whose gradient is denoted by $g_x = \nabla f(x_k)$, the iteration method that the conjugate gradient (CG) method uses in it of the line search is:

$$x_0 \epsilon R^n, \quad x_{k+1} = x_k + \alpha_k d_k \tag{2}$$

where α_k is the step size, in order to ensure the new method's global convergence, we will impose that the step length α_k satisfies the Wolfe conditions which have a good property to prove convergence for more detail see [1]-[6]:

$$f(x_k + \alpha_k d_k) - \mathrm{f}(x_k) \leq \sigma_1 \alpha\, g_k^T\, d_k \tag{3}$$

$$g(x_k + \alpha_k d_k)^T \geq \sigma_2\, g_k^T\, d_k \tag{4}$$

where $0 < \sigma_1 < \sigma_2 < 1$ see [7] and d_k is the search direction generation by:

$$d_{k+1} = -g_{k+1} + \beta_k d_k \tag{5}$$

where β_k is the CG update parameter, which is a scalar. It's worth noting that the formula specification of the update parameter is a critical component of any CG algorithm, which is why different CG algorithms have been proposed to conform to different choices of β_k in (5). In [8]-[13], the parameters are given by:

$$\beta_k^{FR} = \frac{g_{k+1}^T\, g_{k+1}}{g_k^T\, g_k} \tag{6}$$

$$\beta_k^{DY} = \frac{g_{k+1}^T\, g_{k+1}}{y_k^T\, d_k} \tag{7}$$

$$\beta_k^{PRP} = \frac{g_{t+1}^T\, y_k}{\|g_k\|^2} \tag{8}$$

$$\beta_k^{HS} = \frac{g_{k+1}^T\, g_{k+1}}{d_k^T y_k} \tag{9}$$

$$\beta_k^{BSQ} = \frac{g_{k+1}^T\, g_{k+1}}{\alpha(\, g_k^T\, d_k)^2 / 2(f_k - f_{k+1})} \tag{10}$$

Furthermore, some CG methods for unconstrained optimization problem are not globally convergent. As a result, the researchers have been working to improve CG methods that are both globally convergent and numerically efficient [14]. We present the motivation and new algorithm of the proposed method. The global convergence of the proposed algorithm is exhibited with distinct quite different computational efficiency.

2. THE PROPOSED METHOD

The conjugacy condition for nonlinear conjugate gradient methods is given by (11).

$$y_k^T d_{k+1} = 0 \tag{11}$$

Perry decided to extend the deadline of (11) as:

$$d_{k+1}^T y_k = -g_{k+1}^T s_k \tag{12}$$

Dai and Liao in [15] took Perry's approach and added a nonnegative parameter t to suggest the following extension of (12).

$$d_{k+1}^T y_k = -t g_{k+1}^T s_k \tag{13}$$

We suggest this modification to the numerator of β_k^{BSQ} [13], update the parameter to obtain:

$$\beta_k^{MBSQ} = \frac{\|g_{k+1}\|^2 + t g_{k+1}^T s_k}{\alpha(\, g_k^T\, d_k)^2 / 2(f_k - f_{k+1})} \tag{14}$$

Following the Li *et al.* approach in [16] and β_k^{MBSQ} we modified the following parameter extension:

$$\beta_k^{MBSQ} = \frac{\|g_{k+1}\|^2}{\alpha(\, g_k^T\, d_k)^2 / 2(f_k - f_{k+1})} + t\,\frac{g_{k+1}^T s_k}{\alpha(\, g_k^T\, d_k)^2 / 2(f_k - f_{k+1})} = \beta_k^{BSQ} + t\,\frac{g_{k+1}^T s_k}{\alpha(\, g_k^T\, d_k)^2 / 2(f_k - f_{k+1})} \tag{15}$$

where t is a nonnegative parameter, whose values have been calculated by the use of the conjugacy condition analysis. More of than we compute t numerically by multiplying search direction by y_k and by using (14) we obtain:

$$y_k^T d_{k+1} = -y_k^T g_{k+1} + \beta_k^{MBSQ} y_k^T d_k \tag{16}$$

Now we substitute $y_k^T d_{k+1} = -t\, g_{t+1}^T s_k$ if the direction is in exact (ILS) and so we have:

$$-t\, g_{k+1}^T s_k = -y_k^T g_{k+1} + \frac{g_{k+1}^T g_{k+1} + t\, g_{k+1}^T s_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})} y_k^T d_k$$

$$-t\, g_{k+1}^T s_k - \frac{(t\, g_{k+1}^T s_k) y_k^T d_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})} = -y_k^T g_{k+1} + \frac{(g_{k+1}^T g_{k+1}) y_k^T d_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}$$

$$t = \frac{y_k^T g_{k+1} - \dfrac{g_{k+1}^T g_{k+1} \quad y_k^T d_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}}{g_{k+1}^T s_k + \dfrac{g_{k+1}^T s_k \; y_k^T d_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}}$$

$$t = \frac{(y_k^T g_{k+1}) \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) - g_{k+1}^T g_{k+1} y_k^T d_k}{g_{k+1}^T s_k\, \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) + g_{k+1}^T s_k\, y_k^T d_k} \tag{17}$$

Substituting the value of t from (17) into (15) yields:

$$\beta_k^{MSQ} = \frac{g_{k+1}^T g_{k+1} + t\, g_{k+1}^T s_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}$$

$$= \frac{g_{k+1}^T g_{k+1} + \dfrac{(y_k^T g_{k+1}) \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) - g_{k+1}^T g_{k+1} y_k^T d_k}{g_{k+1}^T s_k\, \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) + g_{k+1}^T s_k\, y_k^T d_k} g_{k+1}^T s_k}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}$$

By taking $g_{k+1}^T s_k$ from the numerator and denominator as common factor:

$$= \frac{g_{k+1}^T g_{k+1} + \dfrac{(y_k^T g_{k+1}) \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) - g_{k+1}^T g_{k+1} y_k^T d_k}{\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k}}{\alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}$$

$$= \frac{g_{k+1}^T g_{k+1} \left(\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k \right) + (y_k^T g_{k+1}) \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1}) - g_{k+1}^T g_{k+1} y_k^T d_k}{[\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k]\; \alpha (g_k^T d_k)^2 / 2(f_k - f_{k+1})}$$

$$= \frac{g_{k+1}^T g_{k+1} \left(\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k - y_k^T d_k \right) + (y_k^T g_{k+1}) * \dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})}}{\left[\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k \right] * \dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})}}$$

$$\beta_k^{MSQ} = \frac{g_{k+1}^T g_{k+1} + y_k^T g_{k+1}}{\dfrac{\alpha (g_k^T d_k)^2}{2(f_k - f_{k+1})} + y_k^T d_k} \tag{18}$$

2.1. Outlines of the new algorithm

Define k=0 and choose an initial point $x_0 \epsilon R^n$

If $\|g_k\| = 0$, then terminate, otherwise proceed next step.

Calculate the descent d_k using (5).

Determine a step size α_k by Wolfe line search condition (3), (4).
Let $x_{k+1} = x_k + \alpha_k d_k$.
Estimate β_k which defined in (18).
Set k=k+1 and proceed to step (2).

3. GLOBAL CONVERGENCE

The following assumption is needed to analyze the algorithm's global convergence.

a) The level set $\xi = \{x \epsilon R^n | f(x) \le f(x_1\}$ is bounded.
b) f(x) is continuously differentiable and its gradient is Lipchitz continuous in some neighborhood u of ξ, that is to say in particular, there exists a constant $p > 0$ such that $\|g(x) - g(y)\| \le \|x - y\| \ \forall\, x, y \epsilon \xi$, more details can be found in [17], The well-known Zoutendijk condition [18] is given by the following lemma.

3.1. Lemma (1)

Assume that assumptions a) and b) are true, and consider any iteration of the form (5), where d_k is the path direction and the step size α_k satisfies the condition (3), (4), then the zoutendijk condition:

$$\sum_{k=1}^{\infty} \frac{(g_k^T d_k)^2}{\|d_k\|^2} < \infty \tag{19}$$

holds.

3.2. Lemma (2)

If d_{k+1} is given in (5) and β_k^{MSQ} is given in (18), the following result holds.

$$g_{k+1}^T d_{k+1} < -c \|g_{k+1}\|^2 \forall k \tag{20}$$

Proof:

We have $d_1 = -g_1$ then $d_1^T g_1 < 0$ this is by induction for k=1, then we conclude that $d_k^T g_k < 0, \forall\, k \ge 2$, [19].

$$g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 + \frac{g_{k+1}^T g_{k+1} + y_k^T g_{k+1}}{\alpha(g_k^T d_k)^2/2(f_k - f_{k+1}) + y_k^T d_k} g_{k+1}^T d_k$$

In [8], It follows from $|g_{k+1}^T d_k| \le -\sigma g_k^T d_k$ that $g_{k+1}^T d_k \le -\sigma g_k^T d_k$ and $d_k^T y_k = d_k^T(g_{k+1} - g_k) \ge (\sigma - 1)\, g_k^T d_k$ and from $d_k^T g_k \le -c\|g_k\|^2$ by using powell restart equation (i.e $|g_k^T g_{k+1}| \ge 0.2 g_{k+1}^2$)

$$g_{k+1}^T d_{k+1} \le -\|g_{k+1}\|^2 + \frac{(\|g_{k+1}\|^2 + \|g_{k+1}\|^2)(-\sigma g_k^T d_k)}{\alpha(g_k^T d_k)^2/2(f_k - f_{k+1}) + (\sigma - 1) g_k^T d_k}$$

$$\le -\|g_{k+1}\|^2 + \frac{-2\|g_{k+1}\|^2 \sigma}{(\alpha(g_k^T d_k)/2(f_k - f_{k+1})) + (\sigma - 1)}$$

From (3) and (4) we have

$$g_{k+1}^T d_{k+1} \le -\|g_{k+1}\|^2 + \frac{-2\sigma \|g_{k+1}\|^2 2(f_k - f_{k+1})}{\alpha(g_k^T d_k) + (\sigma - 1)(2(f_k - f_{k+1}))}$$

$$\le -\|g_{k+1}\|^2 + \frac{2\sigma \|g_{k+1}\|^2 2(f_{k+1} - f_k)}{\alpha(g_k^T d_k) + (\sigma - 1)(2(f_k - f_{k+1}))}$$

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

$$\le -\|g_{k+1}\|^2 + \frac{2\sigma \|g_{k+1}\|^2 (2\delta)}{1 + (\sigma - 1)(-2\delta)}$$

Let $\ell = \frac{2\sigma\,(2\delta)}{1+(\sigma-1)(-2\delta)}$ and $0<\ell<1$, then we have $g_{k+1}^T\, d_{k+1} \le -\,\|g_{k+1}\|^2 + \ell\|g_{k+1}\|^2$

$$\therefore\; g_{k+1}^T\, d_{k+1} \le -\,c\,\|g_{k+1}\|^2 \tag{21}$$

By this mathematical induction, we reach the result.

3.3. Lemma (3)

Assume that x_1 is a starting point for which assumption a) is hold. If the new method generates x_1, x_2, x_3 , and so on then,

$$\lim_{k\to\infty} inf\,\|g_k\| = 0 \tag{22}$$

Proof: Assume that the inference is false, that is, there is an appositive constant such that $\|g_k\| \ge \rho$ for all k, since

$d_{k+1} = -g_{k+1} + \beta_k d_k$ which can be written as

$$d_{k+1} + g_{k+1} = \beta_k d_k \tag{23}$$

and since

$\beta_k = \frac{g_{k+1}^T\, g_{k+1} + y_k^T g_{k+1}}{\alpha(\, g_k^T\, d_k)^2/2(f_k - f_{k+1}) + y_k^T\, d_k}$ and from Wolfe condition (3), (4)

$f_k - f_{k+1} \ge -\delta\alpha\, g_k^T d_k$and from $d_k^T y_k \ge (\partial - 1) g_k^T d_k$ [8]

$$\therefore \beta_k \le \frac{2\,\|g_{k+1}\|^2 \quad .2(f_k - f_{k+1})}{\alpha(\, g_k^T\, d_k)^2 + 2\, y_k^T\, d_k\, (f_k - f_{k+1})}$$

$$\le \frac{2\|g_{k+1}\|^2 \quad .2(f_k - f_{k+1})}{\alpha(\, g_k^T\, d_k)^2 + \, 2\, y_k^T\, d_k\, \;(-\delta\alpha\, g_k^T d_k)}$$

$$\le \frac{2\|g_{k+1}\|^2 \quad .(-2)(f_{k+1} - f_k)}{\alpha(\, g_k^T\, d_k)^2 + \, 2\, y_k^T\, d_k\, \;(-\delta\alpha\, g_k^T d_k)}$$

$$\le \frac{2\,\|g_{k+1}\|^2 \quad .-(2\alpha\delta\, g_k^T d_k)}{\alpha(\, g_k^T\, d_k)^2 + \, 2(\sigma-1)\, g_k^T\, d_k\, (-\delta\alpha\, g_k^T d_k)}$$

$$\le \frac{-4\,\|g_{k+1}\|^2 \quad .\alpha\delta}{g_k^T\, d_k[\alpha + \, 2(\sigma-1) - \delta\alpha]}$$

$$\le \frac{-4\,\|g_{k+1}\|^2 \quad .\alpha\delta}{-\,\|g_k\|^2[\alpha + 2(\sigma-1) - \delta\alpha]} \tag{24}$$

$\therefore |\beta_k| < j$ such that j is constant

$$\|d_{k+1}\| = \|-g_{k+1}\| + |\beta_k|\|d_k\|$$

$$\le \|-g_{k+1}\| + |j|\|d_k\|$$

$$\le £ + |j|\ell \tag{25}$$

and we concluding the proof with this contradiction that is:

$$\sum_{i=1}^{k} \frac{1}{\|d_k\|^2} \ge \frac{1}{(£ + |j|\ell)^2} \sum 1 = \infty \tag{26}$$

Which is contradiction with zoutendijk theorem therefore the algorithm is globally convergent.

4. RESULT AND DISCUSSION

Now, we preset the arithmetical experiments we test and compare our method with B_k^{HS}, the code is written in using Fortran 90 to apply these methods and the test function are selected from [20]. The stopping state is defined as $\|g_{k+1}\| \leq 10^{-6}$ as recommended by [21]. We used 14 test problems with dimension 100 and 1000. The computation results shown in Table 1 have the following meaning: the total number of iterations (NOI), the total number of restarts (NOR), and the total number of function evaluations (NOF). Also, Table 2 shows the average efficiency of the new algorithm with respect to harmony search (HS) method. Furthermore, optimization problems used in many papers for example, see [22]-[25].

Table 1. Numerical results of new algorithms and HS-CG algorithm

Test Function	n	New Formula			HS		
		NOI	NOR	NOF	NOI	NOR	NOF
Quadratic Diagonal Perturbed	100	48	11	86	52	10	90
	1000	167	31	291	171	36	302
Trigonometric	100	18	9	34	19	10	36
	1000	38	22	68	33	19	64
Extended Beale	100	12	7	24	14	8	27
	1000	14	9	27	15	10	29
Extended Himmelblau	100	10	6	19	10	6	19
	1000	10	6	19	11	6	21
HIMMELBH (CUTE)	100	6	3	13	6	3	13
	1000	6	3	13	6	3	13
Broyden Tridiagonal	100	29	6	50	28	5	50
	1000	34	13	59	38	17	61
Almost Perturbed Quadratic	100	90	25	141	112	40	175
	1000	283	78	448	346	106	547
EDENSCH (CUTE)	100	28	10	51	38	22	466
	1000	34	18	230	44	27	617
DIXON3DQ (CUTE)	100	432	120	689	487	139	762
	1000	2001	551	3181	2001	543	3160
DENSCHNA (CUTE)	100	9	6	17	9	6	17
	1000	9	6	18	9	6	18
DENSCHNC (CUTE)	100	14	9	27	13	9	24
	1000	4	10	27	12	9	24
DENSCHNB (CUTE)	100	7	5	15	7	5	15
	1000	7	5	15	7	5	15
DENSCHNF (CUTE)	100	26	22	42	24	19	41
	1000	20	16	37	28	23	47
BIGGSB1 (CUTE)	100	423	116	673	551	156	868
	1000	2001	552	3155	2001	579	3155
Total		5780	1675	9469	6092	1827	10676

Table 2. Average efficiency of the new algorithm

	HS algorithm	New Formula algorithm
NOI	100%	94.88%
NOR	100%	91.68%
NOF	100%	88.69%

5. CONCLUSION

A new CG-method based on the conjugacy condition have been derived with a new update parameter, which is demonstrated the theory of global convergence for one of the proposed methods under reasonable assumptions. According to numerical results, the proposed algorithms has outperformed the regular HS method on average. Furthermore, the efficiency of new algorithm has been explained clearly based on arithmetic results.

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