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New Spectral Idea for Conjugate Gradient Methods and Its Global Convergence Theorems

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Abstract. Recently, the unconstrained optimization conjugate gradient methods have been widely utilized, especially for problems that are known as large-scale problems. This work proposes a new spectral gradient coefficient obtained from a convex linear combination of two different gradient coefficients to solve unconstrained optimization problems. One of the most essential features of our suggested strategy is to guarantee the suitable subsidence direction of the line search precision. Furthermore, the proposed strategy is more effective than previous conjugate gradient approaches and stationery, which have been observed in the test problem. However, when it is compared to other conjugate gradient methods, such as FR methods, the proposed method confirmed the globally convergent, indicating that it can be used in scientific data computation.

2020 Mathematics Subject Classifications: 65K10

Key Words and Phrases: Conjugate gradient, Spectral, Unconstrained optimization, Global convergence, Descent property

1. Introduction

The spectral gradient approaches presented by Barzilai and Browein [5] and later researched by Raydan [23] have proven to be useful and valuable in this area, which are utilized to determine the local minimizers of large-scale problems [2]. In this paper, we describe a spectral gradient technique to solve unconstrained optimization problems of the form:

$$\min_{x \in R} f(x) \tag{1}$$

In most cases, the conjugate gradient approach creates a sequence $\{x_k\}$ in such a way:

$$x_{k+1} = x_k + \alpha_k d_k \tag{2}$$

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For $k = 0$, x_0 denotes the starting position, α_k denotes the specified step size by a line search, d_k signifies the direction of search, which is specified by:

$$d_{k+1} = -g_{k+1} + \beta_k d_k \tag{3}$$

where $d_0 = -g_0$ for $k = 0$ and β_k is a scalar, g_{k+1} refers to the gradient $\nabla f(x_{k+1})$ at the new point. The most familiar β_k formulation is the Fletcher-Reeves (FR), Polak-Ribire, Hestenes-Stiefel (HS), Dai and Yan (DY) formulations which are supplied by: see [12][20][21][17][6]

$$\beta_k^{FR} = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \tag{4}$$

$$\beta_k^{PRP} = \frac{g_{k+1}^T y_k}{||g_k||^2} \tag{5}$$

$$\beta_k^{HS} = \frac{g_{k+1}^T \; g_{k+1}}{d_k^T y_k} \tag{6}$$

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

Also, recently, Hassan [13] suggests a new formula which is denoted in equations (8), (9) respectively.

$$\beta_k^{Y} = \frac{g_{k+1}^T y_k}{(f_k - f_{k+1})/\alpha_{k} - g_k^T d_k/2} \tag{8}$$

$$\beta_k^{G} = \frac{g_{k+1}^T g_{k+1}}{(f_k - f_{k+1})/\alpha_{k} - g_k^T d_k/2} \tag{9}$$

Where the last two equations of β_k are used to suggest a new form of β_k, which we call β_k^{NN}. The other β_k parameters have been offered in the literature see for example [1][3][4][10][11]. To avoid the non-convergence in the nonlinear function which is used with inexact line search the following condition is used:

$$\left|g_{k+1}^T g_k\right| > 0.2||g_{k+1}|| \tag{10}$$

Known as the Powell restart condition [7]. Also, to avoid the negative case of β_k we use Wolfe conditions to guarantee the convergence of non-linear conjugate methods for the research [24]. More information on these line search methods can be found in the literature [8][19][26][27]

$$f(x_k + \alpha_k d_k) \leq f(x_k) + \delta_1 \alpha_k d_k^T g_k \tag{11}$$

$$g(x_k + \alpha_k d_k)^T d_k \geq \delta_2 \alpha_k d_k^T g_k \tag{12}$$

Where d_k is descant direction, $g_k^T d_k < 0$, and $0 < \delta_1 < \delta_2 < 1$. Dai and Yuan [6] show that the FR method satisfies the global convergence feature if the strong Wolfe conditions are satisfied. Recently, combining the well numerical results execution of PRP and HS with the globally convergent properties of the FR and DY methods [6], are the way that is adopted in this paper, which will be discussed in the second section. the systematic sequence of this paper is: The second section proposes a new spectral CG formula and the section three establishes the new method's global convergence. The numerical experiments are shown in the fourth Section, and finally, the fifth Section presents the comparison of the results and conclusion.

2. New Spectral formula for CG Method

The new concept is to redirect the search path so that the new path guarantees the condition.

$$g_{k+1}^T\, d_{k+1} \le -c\, ||g_{k+1}||^2 \tag{13}$$

Zhang et al. [28] suggested a conjugate gradient approach based on the modification of the Fletcher-Reeves method in such a way that the direction d_k which is given by [14]:

$$d_{k+1} = -\theta g_{k+1} + \beta_k\, d_k \tag{14}$$

and the scalar θ is defined as, $\theta = \left(1 + \beta_k \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2}\right)$
Now to improve the proposed CG method, we combine the good computational properties of β_k^Y and β_k^G method which is given in equations (8) and (9) respectively. These methods have strong convergence properties, then rewrite the new formula of β_k as a linear combination of (8) and (9), therefor our new formula β_k^{NN} becomes:

$$\beta_k^{NN} = (1-r)\,\beta_k^Y \; + r\;\beta_k^G \tag{15}$$

Where $0 < r < 1$, $\beta_k^Y = \frac{g_{k+1}^T\; y_k}{(f_k - f_{k+1})/\alpha_k - \; g_k^T\; d_k/2}$, and $\beta_k^G = \frac{g_{k+1}^T\quad g_{k+1}}{(f_k - f_{k+1})/\alpha_k - \; g_k^T\; d_k/2}$

Now by multiplying (14) by y_k^T and using the Conjugacy condition [25] $y_k^T\, d_{k+1} = 0$ in order to compute the value of r we get:

$$y_k^T\;(-\theta g_{k+1} + \beta_k\; d_k) = 0 \tag{16}$$

$$-[1 + \beta_k \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2}] y_k^T\, g_{k+1} + \beta_k y_k^T\, d_k = 0 \tag{17}$$

By using (15) we get:

$$-\left[1 + [(1-r)\,\beta_k^Y \, + r\beta_k^G\right] \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2}] y_k^T\, g_{k+1} + [(1-r)\,\beta_k^Y \, + r\beta_k^G] y_k^T d_k = 0$$

$$r\left[-\beta_k^G \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2} y_k^T\, g_{k+1} + \beta_k^Y \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2} y_k^T\, g_{k+1} - \beta_k^Y y_k^T\, d_k + \beta_k^G y_k^T\, d_k\right]$$

$$= \beta_k^Y \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2} y_k^T\, g_{k+1} - \beta_k^Y y_k^T\, d_k + y_k^T\, g_{k+1}$$

$$\therefore r = \frac{\beta_k^Y \left(\frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2} y_k^T\, g_{k+1} - y_k^T\, d_k \right) + y_k^T\, g_{k+1}}{\left(\beta_k^G - \beta_k^Y\right) \left(y_k^T\, d_k - \frac{d_k^T\, g_{k+1}}{||g_{k+1}||^2} y_k^T\, g_{k+1} \right)} \tag{18}$$

This is the final form of r which is denoted in the equation above. the explanation of the outlines of the new algorithm might be stated as follows:

2.1. The NN-CG Algorithm

- 1^{st}: take $x_1 \in R^n, \varepsilon > 0, d_1 = -g_1$ if $||g_1|| < \varepsilon$, then quit.
- 2^{nd}: if $||g_{k+1}|| < \varepsilon$ then come to the end; otherwise proceed to 3^{th} step.
- 3^{rd}: By satisfying Wolfe conditions (11) and (12), find α_k and take $x_{k+1} = x_k + \alpha_k d_k$
- 4^{th}: find β_k by equation (15), then compute d_{k+1} by (3).
- 5^{th}: put $k = k + 1$, go-to 2^{nd} .

3. The Global Convergence Theorem and hypothesis

The following hypothesis is required to investigate a new convergence method:

`hypothesis number one:`

(i) The set $\Omega = x \in R^n | f(x) \leq f(x_0)$ is bounded when $x_0 \in R^n$, is an initial point.

(ii) There exists a constant W>0 in an open convex set N that includes f is continuously differentiable and the gradient that satisfies Lipschitz condition is continuous. For more detail see [29]. Such as:

$$||g\,(x) - g(y)|| \leq W||x - y||, \quad \forall x, y \in \Omega \tag{19}$$

Furthermore, we can deduce from the hypothesis that p and $\ell > 0$ are constants such that:

$$||x|| \leq p, \quad ||g(x)|| < \ \ell \ , \in \Omega$$

Lemma 1. *Consider that hypothesis number one is holding, and let any step of the type (3) where d_k is decline direction and α_k fulfills conditions (11) and (12), so Zoutedijk condition hold. [30][22].*

$$\sum_{k=1}^{\infty} \frac{\left(g_k^T d_k\right)^2}{||d_k||^2} < \infty \tag{20}$$

Following that, we present additional lemmas that are critical for the global convergence dissection.

Lemma 2. *Suppose that hypothesis number one holds, and take into account any iteration of the form (2) then the direction* d_{k+1} *which is given in (14) satisfies the sufficient descant condition*

$$d_{k+1}^T\ g_{k+1} = -||g_{k+1}||^2 \tag{21}$$

Proof. From (15), for $k = 0$ the result is hold and we have $d_1^T g_1 = -||g_1||^2$, now when $k > 0$ we obtain:

$$\begin{aligned} g_{k+1}^T\ d_{k+1} &= -\left(1 + \beta_k \frac{g_{k+1}^T d_k}{||g_{k+1}||^2}\right) ||g_{k+1}||^2 + \beta_k g_{k+1}^T d_k \\ = -||g_{k+1}||^2 - \beta_k &\frac{g_{k+1}^T\ d_k}{||g_{k+1}||^2} . ||g_{k+1}||^2 + \beta_k g_{k+1}^T\ d_k = -||g_{k+1}||^2 \end{aligned} \tag{22}$$

We see that (21) holds for all $k > 0$. So, the **proof** is complete.

Lemma 3. *Consider that hypothesis (1) and (2) hold and let* α_k *satisfies Wolfe's condition (11), (12) then* β_k *which is determined by (15) satisfies* $0 < \beta_k$

Proof. from the line of inquiry condition (11), (12) as well as the sufficient descent condition (21), and since $d_k^T g_k = -||g_k||^2$ it is possible to show that:

$$\beta_k^Y = \frac{g_{k+1}^T y_k}{(f_k - f_{k+1})/\alpha_k - g_k^T d_k/2} > \frac{||g_{k+1}||^2 - g_{k+1}^T g_k}{-\delta_1 d_k^T g_k + \frac{||g_k||^2}{2}} \tag{23}$$

$$\begin{aligned} \beta_k^G = \frac{g_{k+1}^T g_{k+1}}{(f_k - f_{k+1})/\alpha_k - g_k^T d_k/2} > \frac{||g_{k+1}||^2}{-\delta_1 d_k^T g_k + \frac{||g_k||^2}{2}} &> \frac{||g_{k+1}||^2}{\delta ||g_k||^2 + \frac{||g_k||^2}{2}} \\ &= \frac{||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right) ||g_k||^2} > 0 \end{aligned} \tag{24}$$

Then from (23), (24) and (15) we have:

$$\beta_k^{NN} = (1 - r)\,\beta_k^Y\ + r\ \beta_k^G$$

$$= (1 - r)\frac{||g_{k+1}||^2 - g_{k+1}^T g_k}{\left(\delta + \frac{1}{2}\right) ||g_k||^2} + r\frac{||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right) ||g_k||^2} = \frac{||g_{k+1}||^2 - g_{k+1}^T g_k + r g_{k+1}^T g_k}{\left(\delta + \frac{1}{2}\right) ||g_k||^2}$$

From Powell restart condition (10) we have

$$\beta_k^{NN} > \frac{||g_{k+1}||^2 - 0.2||g_{k+1}||^2 + 0.2r||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right)||g_k||^2} > \frac{0.8||g_{k+1}||^2 + 0.2r||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right)||g_k||^2}$$
$$\therefore \beta_k^{NN} = \frac{n||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right)||g_k||^2} > 0 \tag{25}$$

by assuming $n = (0.8 + 0.2r)$, and since $0 < r < 1$ then it is clearly that $\beta_k^{NN} > 0$

Theorem 1. *Assume that hypothesis number one is true, $\{x_k\}$ is a sequence generated by the algorithm (2.1) and α_k fulfill the Wolfe's conditions (11) and (12), Then we need to prove that* $\lim_{k\to\infty} inf||g_{k+1}|| = 0$

Proof. we use the disagreement method to complete the proof which assumes that $||g_{k+1}|| > \gamma$ for $\gamma > 0$ from (3) it follows that: $d_{k+1} + g_{k+1} = \beta_k d_k$ by squaring the equation (3) we have:

$$||d_{k+1}||^2 + 2g_{k+1}^T d_{k+1} + ||g_{k+1}||^2 = \beta_k^2||d_k||^2$$

Since the sufficient descant condition (21) is held, we obtain:

$$\begin{aligned} ||d_{k+1}||^2 &= (\beta_k)^2||d_k||^2 - ||g_{k+1}||^2 - 2g_{k+1}^T\ d_{k+1} \\ &= (\beta_k)^2||d_k||^2 - ||g_{k+1}||^2 + 2||g_{k+1}||^2 \\ &= (\beta_k)^2||d_k||^2 + ||g_{k+1}||^2 \end{aligned} \tag{26}$$

Both sides are divided by $\left(g_{k+1}^T\ d_{k+1}\right)^2$ we have:

$$\begin{aligned} \frac{||d_{k+1}||^2}{\left(g_{k+1}^T d_{k+1}\right)^2} &\leq \left(\beta_k^2\right)\frac{||d_k||^2}{\left(g_{k+1}^T d_{k+1}\right)^2} + \frac{||g_{k+1}||^2}{\left(g_{k+1}^T d_{k+1}\right)^2} \\ &\leq (\beta_k)^2\frac{||d_k||^2}{\left(g_{k+1}^T d_{k+1}\right)^2} + \frac{1}{||g_{k+1}||^2} \end{aligned} \tag{27}$$

Now from (25), (27) we obtain:

$$\begin{aligned} \frac{||d_{k+1}||^2}{\left(g_{k+1}^T d_{k+1}\right)^2} &\leq \left(\frac{n||g_{k+1}||^2}{\left(\delta + \frac{1}{2}\right)||g_k||^2}\right)^2\frac{||d_k||^2}{||g_{k+1}||^4} + \frac{1}{||g_{k+1}||^2} \\ &= \frac{n^2||d_k||^2}{\left(\delta + \frac{1}{2}\right)^2||g_k||^4} + \frac{1}{||g_{k+1}||^2} \\ &= \frac{n^2||d_k||^2}{\left(\delta + \frac{1}{2}\right)^2\left(g_k^T d_k\right)^2} + \frac{1}{||g_{k+1}||^2} \end{aligned} \tag{28}$$

Since that:

$$\frac{||d_1||^2}{(g_1^T d_1)^2} = \frac{1}{||g_1||^2} \tag{29}$$

From this and $||g_{k+1}|| > \varepsilon^2 \;\; \forall k$ we have:

$$\frac{||d_{k+1}||^2}{(g_{k+1}^T d_{k+1})^2} \leq \sum_{i=1}^{k+1} \frac{1}{(\delta + 1/2)^2 ||g_i||^2} \leq \frac{k}{(\delta + 1/2)^2 \varepsilon^2}$$

$$\therefore \frac{(g_{k+1}^T d_{k+1})^2}{||d_{k+1}||^2} \geq \frac{(\delta + 1/2)^2 \varepsilon^2}{k}$$

Which indicates:

$$\sum_{k=1}^{\infty} \frac{(g_{k+1}^T d_{k+1})^2}{||d_{k+1}||^2} \geq \sum_{k=1}^{\infty} \frac{(\delta + \frac{1}{2})^2 \varepsilon^2}{k} = \infty \tag{30}$$

And this is in direct opposition to the Zoutendijk condition (20), with this contradiction we complete **proof**.

4. Numerical Experiments

Now we set up the numeral experiments, Compute and make a comparison between our method vs. β_k^{FR}. The comparison is written using the Fortran 90 program, and the test function is implemented using the functions chosen from Andrei [2]. The measure of stooping the algorithm is denoted as $||g_{k+1}|| \leq 10^{-6}$, We use 27 test problems with different dimensions to experiment with the execution of the new method. Table 1 shows the calculation result, with NOI, NOR, and NOF which stand for the amount of iterations total, restart, and function evaluation, respectively. While Table 2 explains the execution percentage of the new method opposite FR method, also the execution was analyzed by the performance profile software which is developed by Dolan and Mor'e [9] which are seen in Figures 1, 2, 3.

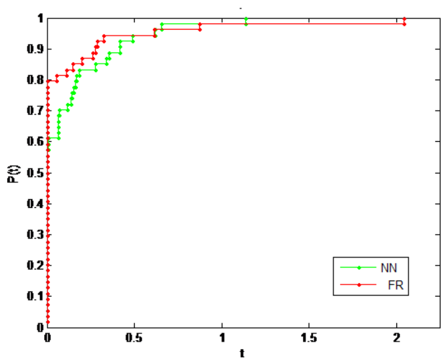

Figure 1: The performance profile of iteration.

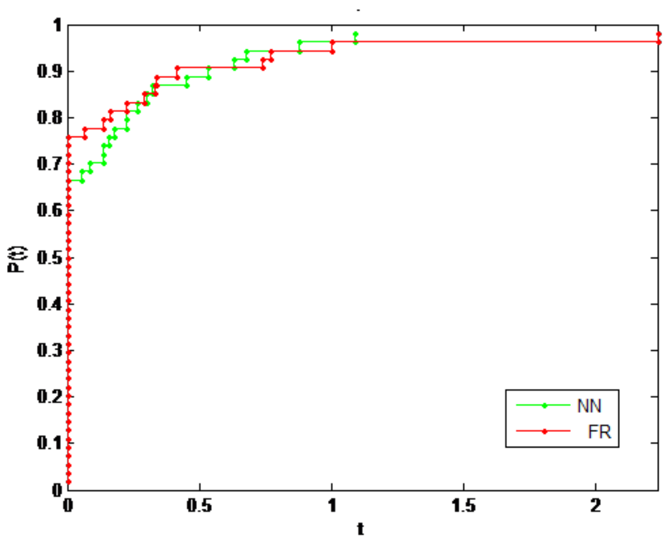

Figure 2: The performance profile of function evaluation.

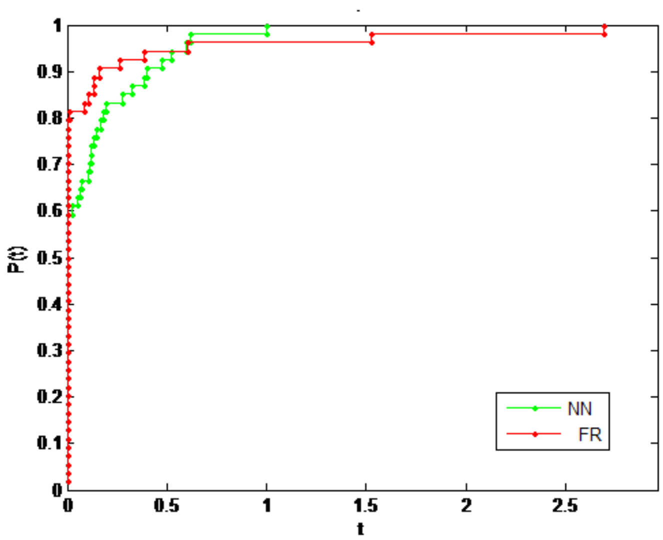

Figure 3: The performance profile of restart.

Test Problem	Dim	NN			FR		
		NOI	NOR	NOF	NOI	NOR	NOF
Trigonometric	100	20	11	37	18	10	34
	1000	33	19	63	40	24	69
Penalty	100	9	6	25	11	6	28
	1000	51	43	959	210	202	6193
Perturbed Quadratic	100	102	35	156	102	31	156
	1000	340	95	559	325	111	494
Raydan 2	100	4	4	9	4	4	9
	1000	4	4	9	4	4	9
Diagonal 2	100	61	18	105	70	24	113
	1000	221	74	377	211	74	351
Generalized Tridiagonal 1	100	23	7	46	22	6	44
	1000	32	17	263	49	29	758
Extended Tridiagonal 1	100	11	6	23	10	5	21
	1000	13	7	26	13	7	26
Generalized Tridiagonal 2	100	42	17	64	37	11	59
	1000	62	25	107	67	28	102
Diagonal 4	100	4	2	8	4	2	8
	1000	4	2	8	4	2	8
Diagonal 5	100	4	4	9	4	4	9
	1000	4	4	9	4	4	9
Extended Himmelblau	100	22	11	38	10	6	19
	1000	12	6	23	22	12	35
Extended PSC1	100	8	6	17	8	6	17
	1000	7	5	15	7	5	15
Extended Powell	100	69	20	129	66	22	127
	1000	100	31	232	89	31	167
Extended BD1	100	63	63	98	63	63	98
	1000	67	67	105	67	67	105
Quadratic Diagonal Perturbed	100	73	9	128	52	11	89
	1000	151	31	268	181	39	321
Extended Wood WOODS	100	32	13	60	25	9	48
	1000	46	16	83	30	13	55
Quadratic QF1	100	95	30	153	85	22	134
	1000	364	111	588	362	101	568
Extended EP1	100	2	2	5	2	2	5
	1000	2	2	5	2	2	5
Extended Tridiagonal 2	100	39	15	63	36	12	57
	1000	42	18	64	40	17	64
NONDIA	100	12	8	23	15	8	30
	1000	12	7	25	9	6	19
DQDRTIC	100	8	1	17	6	1	13
	1000	11	0	23	7	1	15
DIXMAANA	100	7	7	14	7	7	14
	1000	7	3	14	7	5	14
DIZMAANB	100	10	10	18	10	10	18
	1000	11	11	19	11	11	19
DIXMAANC	100	13	13	24	13	13	24
	1000	14	14	25	14	14	25
DIXMAANE	100	79	28	119	82	27	126
	1000	216	67	344	239	60	378
Partial Perturbed Quadratic	100	85	26	135	77	26	120
	1000	250	65	410	249	68	412
Broyden Tridiagonal	100	38	16	58	30	10	48
	1000	40	17	68	33	8	63
Total		3051	1149	6272	3165	1303	11767

Table 1: Results for the NN and FR algorithm

	FR	NN
NOI	100%	96.398%
NOR	100%	88.18%
NOF	100%	53.30%

Table 2: Efficiency of the NN method

5. Conclusion

In this paper, we searched for a new conjugate gradient method that depends on the spectral strategy. We established, under acceptable assumptions, that the global convergence for one of the offered approaches is satisfied. The arithmetical computation explained in Table 1 shows the efficiency of the proposed algorithm outperformed the regular FR method on average, according to the numerical results and Figures 1, 2, 3, which are denoted by the performance profile iteration and the number of function evaluations and CPU time respectively. Furthermore, there are exist many good progress in conjugate gradient algorithms see for example [16][15][18]

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