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Modified Conjugate Gradient Algorithm of Unconstrained Optimization

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Abstract: C*onjugate gradient methods are extremely useful for solving large-scale unconstrained optimization problems. The parameter conjugate is the primary focus of conjugate gradient methods. The current paper proposes new conjugate gradient type parameter methods for solving large-scale unconstrained optimization problems. In this study, a Hessian approximation in diagonal matrix form was used on the basis of a third-order Taylor series expansion. The proposed algorithm's sufficient descent property is established. The new method was globally converged. This new algorithm is found to be competitive with the Fletchers-Reeve algorithm (FR).*

Keyword: *Conjugacy Coefficient; Conjugate gradient; Global convergence; Unconstrained optimization;*

1. PRAFACE

The conjugate gradient methods have been interested in for two reasons, the first is that these methods are among the oldest and best-known techniques for solving systems of linear equations with large dimensions, and the second reason is that these methods can be adapted to solve nonlinear optimization problems.

These methods have advantages that place them between the steep descent method (SD) and Newton's method, because these methods require calculating the first derivatives only, and do not need to calculate and store the second derivatives needed by Newton's method, and it is faster than the steep regression method, that is, it overcomes the slow convergence of these The method, since it does not need to calculate Hessian matrix or any of its approximations, is widely used to solve large scale optimization problems[30].

2. CONJUGTE GRADIENT METHOD

Unconstrained and nonlinear optimization problems are defined as:

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

Since $f(x): R^n \to R$ is a continuous and differentiable function. The conjugate gradient method solves these problems and is efficient in solving them on a large scale due to its simplicity and low storage. The nonlinear conjugated gradient method generates a sequence $\{x_k\}$ starting from the initial point $x_0 \in R^n$ using the frequency defined by the following equation [4].

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

where λ_k is the step size and d_k is the direction of the search identifier

$$d_k = \begin{Bmatrix} -g_{k,} & k = 0 \\ -g_k + \beta_k d_{k-1} & k \geq 0 \end{Bmatrix} \tag{3}$$

where g_k is the conjugate gradient symbol and β_k is the conjugate coefficient, some examples of known β_k are Hestense – Stiefel (HS) [16], Fletcher and Reevs (FR) [10], Polak and Ribiere (PRP) [21], Dai- Yaun (DY) [7], Conjugate Descent (CD) [11], The following are the corresponding formulas for the β_k mentioned:

$$\beta_k^{HS} = \frac{g_{k+1}^T y_k}{d_k^T y_k} \tag{4}$$

$$\beta_k^{FR} = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \tag{5}$$

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

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

$$\beta_k^{CD} = \frac{g_{k+1}^T g_{k+1}}{d_k^T g_k} \quad (8)$$

These CG coefficients could likewise be divided into two groups. The first group comprises of HS, and PR, while in the second group we have FR, DY and CD. It is easy to see that the first group possesses the restart properties, hereas the second group does not have this characteristic [24-25]. In [5] has arranged the CG method into three distinct groups; the classical CG method, the scaled CG method and lastly the hybrid and parameterized CG methods. The classical CG method is the simplest and most straightforward to apply. However, it is difficult to find and produces a new CG method of this type [16].

All of these methods are equivalent if the objective function is strictly convex quadratic, as indicated by [6-7]. However, they differ when applied to general non-quadratic functions. According to [8], the history of CG methods begins with [16], who proposed the first CG method to solve a linear system of equations with a symmetric positive definite matrix. The CG method was then applied to general unconstrained optimization problems in [10]. CG methods are now recognized as extremely valuable for solving large-scale unconstrained optimization problems because they do not require the storage of matrices [1-3,13-15, 17-19, 20, 22, 26-29, 32-34].

3. DERIVING NEW CONJUGACY COEFFICIENTS

Hassian and Taha in 2019 proposed a quasi-Newton condition of the higher order tensor model [17] by making a modification and taking the third order tensor model defined in [16] we get equations from (9) to (12)

$$S_k^T B_{k+1} S_k = S_k^T Y_k + 6(f_k - f_{k+1}) + 3(g_{k+1} + g_k)^T S_k \quad (9)$$

Dividing by n

$$\frac{1}{n} S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{6}{n}(f_k - f_{k+1}) + \frac{3}{n}(g_{k+1} + g_k)^T S_k \quad (10)$$

From above equation we get

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{6}{n}(f_k - f_{k+1}) + \frac{3}{n}(g_{k+1} + g_k)^T S_k - \frac{n-1}{n} g_k^T S_k \quad (11)$$

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{6}{n}(f_k - f_{k+1}) + \frac{3}{n}(g_{k+1} + g_k)^T S_k - \frac{n-1}{n} g_k^T S_k \quad (12)$$

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{6}{n}(f_k - f_{k+1}) + \frac{3}{n} g_{k+1}^T S_k + \frac{3}{n} g_k^T S_k - \frac{n-1}{n} g_k^T S_k \quad (13)$$

Dehghani and others in 2019 knew the following relationship [9]:

$$f_{k+1} - f_k = \int_0^1 \nabla f(x_k + t s_k) dt s_k \cong s_k^T g_k = g_k^T S_k \quad (14)$$

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k - \frac{6}{n} g_k^T S_k + \frac{3}{n} g_{k+1}^T S_k + \frac{3}{n} g_k^T S_k - \frac{n-1}{n} g_k^T S_k \quad (15)$$

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{3}{n} g_{k+1}^T S_k - \frac{2+n}{n} g_k^T S_k \quad (16)$$

Consider B_{k+1} is an approximation of the Hessian matrix $\nabla^2 f(x)$ of the $f(x)$

$$S_k^T B_{k+1} S_k = \frac{1}{n} S_k^T Y_k + \frac{3}{n} g_{k+1}^T S_k - \frac{2+n}{n} g_k^T S_k \quad (17)$$

The quasi –newton condition based on the above relation as follow

$$B_{k+1} S_k = \frac{1}{n} Y_k + \frac{\frac{3}{n} g_{k+1}^T S_k - \frac{2+n}{n} g_k^T S_k}{S_k^T v_k} v_k \quad (18)$$

$$B_{k+1} = \frac{\frac{1}{n} S_k^T Y_k + \frac{3}{n} g_{k+1}^T S_k - \frac{2+n}{n} g_k^T S_k}{S_k^T S_k} \quad (19)$$

From direction newton method

$$d_{k+1}^N = -B_{k+1}^{-1} g_{k+1} \quad (20)$$

Multiply Y_k^T by we get

$$Y_k^T d_{k+1}^N = -B_{k+1}^{-1} Y_k^T g_{k+1} \quad (21)$$

$$Y_k^T(-g_{k+1} + \beta_k d_k) = -B_{k+1}^{-1} Y_k^T g_{k+1} \quad (22)$$

$$(-Y_k^T g_{k+1} + \beta_k Y_k^T d_k) = -B_{k+1}^{-1} Y_k^T g_{k+1} \quad (23)$$

$$\beta_k(Y_k^T d_k) = Y_k^T g_{k+1} - B_{k+1}^{-1} Y_k^T g_{k+1} \quad (24)$$

$$\beta_k = \frac{Y_k^T g_{k+1} - B_{k+1}^{-1} Y_k^T g_{k+1}}{Y_k^T d_k} \quad (25)$$

$$\beta_k = \frac{(1 - B_{k+1}^{-1}) Y_k^T g_{k+1}}{Y_k^T d_k} \quad (26)$$

$$\beta_k = \frac{\left(1 - \frac{S_k^T S_k}{\frac{1}{n} S_k^T Y_k + \frac{3}{n} g_{k+1}^T S_k - \frac{2+n}{n} g_k^T S_k}\right) Y_k^T g_{k+1}}{Y_k^T d_k} \quad (27)$$

3.1 Outline of the Proposed Algorithm (Modification Conjugate Gradient (MCG))

Step 1: Choose an initial value $x_1 \in R^n$, put $\epsilon > 0$, and n.

Step 2: $d_k = -g_k$

Step 3: Calculate the length of the step $\alpha_k > 0$

Step 4: Calculate

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

If it is $\|g_{k+1}\| \leq \epsilon$, then stop.

Step 5: Calculate β_k from equation (27) and Generate

$$d_{k+1} = -g_{k+1} + \beta_k d_k \quad (29)$$

the trend.

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Step 6: If it is $k = n$ go to step 2 otherwise continue.

Step 7: Place $k = k + 1$ and go to step 3.

3.2 The Convergence Analysis

Theoretical Properties for the New CG-Method. In this section, we demonstrate the global convergence of a new algorithm under the following assumption, which has frequently been used in conjugate gradient method convergence analysis.

Assumptions (1)

f is bounded on the set $s = \{x \in R^n : f(x) \le f(x_0)\}$

f is continuously differentiable, the gradient ∇f is Lipchitz continues and there exist constant $L > 0$ such that

$\|\nabla f(x) - \nabla f(y)\| < L\|x - y\|$ for all $x, y \in s$

3.3 Sufficient Descent property

We will show that in this section the proposed algorithm that defined in the equations (28) and (29) satisfy the sufficient descent property that satisfy the convergence property.

Theorem (1)

The search direction d_k ,that generated by the proposed algorithm of modified CG satisfy the descent property for all k , when the step size λ_k satisfied the Wolfe conditions

$$f(x_k + \lambda_k d_k) - f(x_k) \le \rho \lambda_k g_k^T d_k \tag{30}$$

$$g(x_k + \lambda_k d_k)^T d_k \ge \sigma g_k^T d_k \tag{31}$$

Proof: The indication is used to demonstrate the descent property , for $k = 0$, $d_0 = -g_0 \Rightarrow d_0^T g_0 = -\|g_0\| < 0$, then we demonstrated that the theorem holds true for $k = 0$, we assume that $\|S_k\| \le \eta$; $\|g_{k+1}\| \le \gamma$; $\|g_k\| \le \Gamma$ and suppose that the theorem holds true for any k i.e $d_k^T g_k < 0$ or $s_k^T g_k < 0$ $since$ $s_k = \lambda_k d_k$,we will now demonstrate that the theorem holds for k+1.

$$d_{k+1} = -g_{k+1} + \beta_k^{new} d_k \tag{32}$$

Multiply both sides of the above equation by g_{k+1} we get

$$g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 + \beta_k^{new} g_{k+1}^T d_k \tag{33}$$

$$g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 + \left(\frac{\left(1 - \frac{s_k^T s_k}{\frac{1}{\lambda} s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k}\right) Y_k^T g_{k+1}}{Y_k^T d_k}\right) g_{k+1}^T d_k \tag{34}$$

$$g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 + \left(\frac{Y_k^T g_{k+1}}{Y_k^T d_k} - \frac{s_k^T s_k}{\frac{1}{\lambda} s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k} \cdot \frac{Y_k^T g_{k+1}}{Y_k^T d_k}\right) g_{k+1}^T d_k \tag{35}$$

$$g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2 = \left(\frac{Y_k^T g_{k+1}}{Y_k^T d_k} - \frac{s_k^T s_k}{\frac{1}{\lambda} s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k} \cdot \frac{Y_k^T g_{k+1}}{Y_k^T d_k}\right) g_{k+1}^T d_k \tag{36}$$

$$g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2 \le \frac{Y_k^T g_{k+1}}{Y_k^T d_k} g_{k+1}^T d_k - \frac{s_k^T s_k}{\frac{1}{\lambda} s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k} \cdot \frac{Y_k^T g_{k+1}}{Y_k^T d_k} g_{k+1}^T d_k \tag{37}$$

By using the relation

$$u^T v = \frac{1}{2}(\|u\|^2 + \|v\|^2) \tag{38}$$

$$g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2 \le \frac{Y_k^T g_{k+1}}{Y_k^T d_k} g_{k+1}^T d_k - \frac{\|S_k\|^2}{\frac{1}{\lambda}\left(\frac{1}{2}(\|S_k\|^2 + \|Y_k\|^2)\right) + \frac{3}{\lambda}\left(\frac{1}{2}(\|g_{k+1}\|^2 + \|S_k\|^2)\right) - \frac{2+\lambda}{\lambda}\left(\frac{1}{2}(\|g_k\|^2 + \|S_k\|^2)\right)} \tag{39}$$

$$g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2 \le \frac{Y_k^T g_{k+1}}{Y_k^T d_k} g_{k+1}^T d_k \tag{40}$$

Dividing by $\|g_{k+1}\|^2$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{Y_k^T g_{k+1} g_{k+1}^T d_k}{Y_k^T d_k \|g_{k+1}\|^2} \tag{41}$$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{Y_k^T g_{k+1} g_{k+1}^T d_k}{\|Y_k\|\|d_k\|\|g_{k+1}\|^2} \tag{42}$$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{Y_k^T d_k \|g_{k+1}\|\|g_{k+1}\|}{\|Y_k\|\|d_k\|\|g_{k+1}\|^2} \tag{43}$$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{Y_k^T d_k \|g_{k+1}\|^2}{\|Y_k\|\|d_k\|\|g_{k+1}\|^2} \tag{44}$$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{Y_k^T d_k}{\|Y_k\|\|d_k\|} \tag{45}$$

$$\frac{\|g_{k+1}\|^2}{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2} \ge \frac{\|Y_k\|\|d_k\|}{Y_k^T d_k} = \delta > 1 \tag{46}$$

$$\frac{g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2}{\|g_{k+1}\|^2} \le \frac{1}{\delta} \tag{47}$$

$$g_{k+1}^T d_{k+1} + \|g_{k+1}\|^2 \le \frac{1}{\delta} \|g_{k+1}\|^2 \tag{48}$$

$$g_{k+1}^T d_{k+1} \le -\|g_{k+1}\|^2 + \frac{1}{\delta} \|g_{k+1}\|^2 \tag{49}$$

$$g_{k+1}^T d_{k+1} \le -\left(1 - \frac{1}{\delta}\right) \|g_{k+1}\|^2 \tag{50}$$

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Let $c = 1 - \frac{1}{\delta}$

$$g_{k+1}^T d_{k+1} \le -c\|g_{k+1}\|^2 \quad (51)$$

3.4 Global Convergence Property

The conclusion of the following lemma is used to prove the global convergence of nonlinear conjugate gradient methods with inexact line search.

Lemma (1)

Suppose assumptions (1) hold and consider any conjugate gradient method (28) and (29), where d_k is a descent direction and λ_k is obtained by the strong Wolfe line search. If $\sum_{k\ge1}^{\alpha} \frac{1}{\|d_k\|^2} = \alpha$ then $\lim_{k\to} inf\|g_k\| = 0$

For uniformly convex functions that satisfy the above assumptions, we can prove that the norm of d_{k+1} given by (29) is bounded above. Assume that the function f is a uniformly convex function, i.e., there exists a constant $\mu \ge 0$ such that for all $x, y \in S$,

$$\left(g(x) - g(y)\right)^T (x - y) \ge \mu\|x - y\|^2 \quad (52)$$

Using lemma 1 the following result can be proved.

Theorem (2)

Suppose that the assumption (1) hold. Consider the algorithm. If tends to zero and there exists nonnegative constant such that $\|g_k\|^2 \ge \eta_1\|S_k\|^2$, $\|g_{k+1}\|^2 \ge \eta_2\|S_k\|$ and f is a uniformly convex function, then then $\lim_{k\to\infty} inf\|g_k\| = 0$

Proof:

$$\beta_k = \frac{\left(1 - \frac{s_k^T s_k}{\frac{1}{\lambda}s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k}\right) Y_k^T g_{k+1}}{Y_k^T d_k} \quad (53)$$

$$|\beta_k| = \left| \frac{\left(1 - \frac{s_k^T s_k}{\frac{1}{\lambda}s_k^T Y_k + \frac{3}{\lambda} g_{k+1}^T s_k - \frac{2+\lambda}{\lambda} g_k^T s_k}\right) Y_k^T g_{k+1}}{Y_k^T d_k} \right| \le$$

$$\frac{\left(1 - \frac{\|s_k\|^2}{\frac{1}{\lambda}\|s_k\|\|Y_k\| + \frac{3}{\lambda}\|g_{k+1}\|\|s_k\| - \frac{2+\lambda}{\lambda}\|g_k\|\|s_k\|}\right)\|Y_k\|\|g_{k+1}\|}{\|Y_k\|\|d_k\|} \quad (54)$$

$$\|Y_k\| \le L\|S_k\| \quad (55)$$

$$\frac{\left(1 - \frac{\|s_k\|^2}{\frac{1}{\lambda}\|s_k\|\|Y_k\| + \frac{3}{\lambda}\|g_{k+1}\|\|s_k\| - \frac{2+\lambda}{\lambda}\|g_k\|\|s_k\|}\right)\|Y_k\|\|g_{k+1}\|}{\|Y_k\|\|d_k\|} \le$$

$$\frac{\left(1 - \frac{\eta^2}{\frac{1}{\lambda}\eta L\eta + \frac{3}{\lambda}\gamma\,\eta - \frac{2+\lambda}{\lambda}\Gamma\eta}\right) L\eta\gamma}{L\eta\frac{\|S_k\|}{\lambda}} \quad (56)$$

$$\|d_{k+1}\| \le \|g_{k+1}\| + |\beta_k|\|S_k\| \quad (57)$$

$$\|d_{k+1}\| \le \gamma + \frac{\left(1 - \frac{\eta^2}{\frac{1}{\lambda}\eta L\eta + \frac{3}{\lambda}\gamma\,\eta - \frac{2+\lambda}{\lambda}\Gamma\eta}\right) L\eta\gamma}{\frac{L\eta}{\lambda}\|S_k\|} \|S_k\| \quad (58)$$

$$= \gamma + \frac{\left(1 - \frac{\eta^2}{\frac{1}{\lambda}\eta^2 L + \frac{3}{\lambda}\gamma\,\eta - \frac{2+\lambda}{\lambda}\Gamma\eta}\right) L\eta\gamma}{\frac{L\eta}{\lambda}} \quad (59)$$

$$\sum_{k\ge1}^{\alpha} \frac{1}{\|d_{k+1}\|^2} = \infty \quad (60)$$

$$\frac{1}{\left(\gamma + \frac{\left(1 - \frac{\eta^2}{\frac{1}{n}\eta^2 L + \frac{3}{n}\gamma\,\eta - \frac{2+n}{n}\Gamma\eta}\right) L\eta\gamma}{\frac{L\eta}{\lambda}}\right)^2} \sum_{k\ge1}^{\infty} 1 = \infty \quad (61)$$

4. DISCUSS THE RESULT

TABLE I A COMPARISON BETWEEN THE STANDARD ALGORITHM AND THE PROPOSED ALGORITHM

	Standard algorithm			Proposed algorithm		
	N=100	N=500	N=1000	N=1000	N=500	N=1000
1	0.148087E-12	0.935806E-12	0.849261E-12	0	0	0
2	0.100197E-11	0.176978E-06	0.314811E-07	0.107508E-15	0.145028E-15	0.116776E-11
3	0.763453E-06	0.897998E-02	0.234504E-04	0.381342E-02	0.462649E-02	0.739798E-02
4	0.186808E-12	0.886394-05	0.107801E-09	0	0	0
5	0.219824E-13	0	0	0	0	0
6	0.376485E-12	0.733350E-13	0.384188E-12	0.733350E-13	0.384188E-12	0.376485E-12
7	0.128686E-13	0.140332E-13	0.679456E-13	0	0	0
8	0.263136E-06	0.541994E-09	0.462105E-09	0.541994E-09	0.462105E-09	0.263136E-06
9	0.377103E-13	0.131362E-12	0.218847E-12	0	0	0
10	0.103081E-05	0.164257E-04	0.753884E-05	0	0	0

Some non-linear and non-constrained functions were selected to compare between the proposed algorithms (MCG) and the standard algorithm (Fletcher-Reeves)), as they were applied to (10) nonlinear functions and all the functions were applied and all cases used the stop scale

$$\|g_{k+1}\| < \epsilon, \quad \epsilon = 10^{-6} \tag{62}$$

Relying on efficiency measures ($fmin$), we have obtained effective results. From a practical point of view, the efficiency of the results obtained has been shown in the tables from (I.), which represents a comparison between the standard algorithm and the proposed algorithms (MCG). On the results of the approach in other proposed algorithms.

5. CONCLUSION

A set of test functions were used (10 test functions) They are shown in the appendix. To observe the results, the numerical results showed that the developed conjugate gradient algorithms proved their efficiency when the comparisons were based on $fmin$.

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