

A new modification of the quasi-newton method for unconstrained optimization

Hamsa Th. Saeed Chilmeran¹, Huda I. Ahmed², Eman T. Hamed³, Abbas Y. Al-Bayati⁴

¹Department of Mathematics, College of Computers Sciences and Mathematics, University of Mosul, Iraq

^{2,3}Department of Operation Researches and Intelligent Techniques, College of Computers Sciences and Mathematics, University of Mosul, Iraq

⁴University of Telafer, Tall' Afar, Iraq

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ABSTRACT

In this work we propose and analyze a hybrid conjugate gradient (CG) method in which the parameter β_k is computed as a linear combination between Hager-Zhang [HZ] and Dai-Liao [DL] parameters. We use this proposed method to modify BFGS method and to prove the positive definiteness and QN-conditions of the matrix. Theoretical trils confirm that the new search directions aredescent directions under some conditions, as well as, the new search directions areglobally convergent using strong Wolfe conditions. The numerical experiments show that the proposed method is promising and outperforms alternative similar CG-methods using Dolan-Mor'e performance profile".

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Corresponding Author:

Huda Isaam Ahmed

Department of Operation Researches and Intelligent Techniques

College of Computers Sciences and Mathematics

University of Mosul, Iraq

Email: huda72@gmail.com

1. INTRODUCTION

The conjugate gradient (CG) method is an efficient and organized tool for solving the large-scale nonlinear optimization problem, due to its simplicity, easiness, and low memory requirements. This method is very popular for mathematician and engineers and those who are interested in solving the large-scale optimization problems. The nonlinear unconstrained optimization.

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad (1)$$

where $f(x): \mathbb{R}^n \rightarrow \mathbb{R}$ is smooth function bounded from below, generates a sequence of points as formula :

$$x_{k+1} = x_k + \alpha_k d_k \quad (2)$$

where α_k is a optimal step computed by line search and d_k are generated as :

$$d_{k+1} = -g_{k+1}; k=0 \quad \text{and} \quad d_{k+1} = -g_{k+1} + \beta_k d_k; \quad \text{for } k \geq 1 \quad (3)$$

In (3), $\beta_k \in \mathbf{R}$ is known as conjugacy coefficient. There are different CG- methods correspond to different choices for the β_k , such as (HS) method [1], FR method [2], PRP method [3, 4] and DY method [5], Also Dai-Liao [6]. Considered the following formula:

$$\beta_k^{DL} = \frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{g_{k+1}^T s_k}{d_k^T y_k}, \quad t > 0 \quad (4)$$

Where $y_k = g_{k+1} - g_k$. As Hager–Zhang [7] proposed the formula:

$$\beta_k^N = \frac{g_{k+1}^T y_k}{d_k^T y_k} - 2 \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \quad (5)$$

where $\|\cdot\|$ denotes the Euclidean norm. And the author introduced a parameter t_k in (5), yielding:

$$\beta_k^{HZ} = \frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \quad (6)$$

Note that when $t_k = 2$ (6) reduce to (5). For more details see [8]. Many authors are studied the convergence of the on top of formulas for years [9-15]. The line search in the CG-algorithms often is based on the standard Wolfe conditions:

$$f(x_k + \alpha_k d_k) - f(x_k) \leq \delta \alpha_k \nabla f(x_k)^T d_k \quad (7a)$$

$$g_{k+1}^T d_k \geq \sigma \nabla f(x_k)^T d_k \quad (7b)$$

The constants are within the period $0 < \delta < \sigma < 1$, for additional details is found in [16, 17]

2. DERIVATION OF A NEW PARAMETER

We have to drive a parameter β_k which is incorporation between (4) and (6),

$$\begin{aligned} \beta_k^{new} &= \varpi_k \left(\frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{g_{k+1}^T s_k}{d_k^T y_k} \right) + (1 - \varpi_k) \left(\frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \right) \\ \beta_k^{new} &= \varpi_k \frac{g_{k+1}^T y_k}{d_k^T y_k} - \varpi_k t \frac{g_{k+1}^T s_k}{d_k^T y_k} + \frac{g_{k+1}^T y_k}{d_k^T y_k} - t \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} - \varpi_k \frac{g_{k+1}^T y_k}{d_k^T y_k} + t \varpi_k \left(\frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \right) \\ \beta_k^{new} &= \frac{g_{k+1}^T y_k}{d_k^T y_k} - \varpi_k t \frac{g_{k+1}^T s_k}{d_k^T y_k} - (1 - \varpi_k) t \frac{\|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \end{aligned} \quad (8)$$

and the direction is defined by:

$$d_{k+1} = -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{d_k^T y_k} - t \varpi_k \frac{g_{k+1}^T s_k}{d_k^T y_k} - (1 - \varpi_k) \frac{t \|y_k\|^2}{d_k^T y_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} \right] d_k$$

Also we can rewrite the above equation by:

$$d_{k+1} = -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{s_k^T y_k} - t \varpi_k \frac{g_{k+1}^T s_k}{s_k^T y_k} - (1 - \varpi_k) \frac{t \|y_k\|^2}{s_k^T y_k} \frac{g_{k+1}^T s_k}{s_k^T y_k} \right] s_k \tag{9}$$

ϖ_k is a scalar parameter ($0 \leq \varpi_k \leq 1$).

Observe that when using exact line searches (ELS), (8) reduce to β_k^{HS} and using inexact line searches (ILS), when $\varpi_k = 1$, (8) reduce to β_k^{DL} and when $\varpi_k = 0$, (8) to β_k^{HZ} .

3. CONVERGENCE ANALYSIS OF NEW METHOD

In this section, we will show the convergent analysis based on the inexact line search by means of Wolfe line search. We will also show that these CG-coefficients will possess sufficient descent conditions and global convergence properties. Under this inexact line search (7a) and (7b). In the following theorem; we discuss the sufficient condition:

3.1. Sufficient descent condition

For the sufficient descent condition, we present the following Theorem,

Theorem 1

Let g_k and d_k be sequences of generated methods by (2),(3) and (8), then (9) achieved and satisfy the sufficient descent property.

Proof:

multiplying (9) by quantity $\left(\frac{g_{k+1}}{\|g_{k+1}\|^2} \right)$ yields:

$$\frac{d_{k+1}^T g_{k+1}}{\|g_{k+1}\|^2} = -1 + \left[\frac{g_{k+1}^T y_k (s_k^T g_{k+1})}{y_k^T s_k \|g_{k+1}\|^2} - t \varpi_k \frac{(g_{k+1}^T s_k)^2}{y_k^T s_k \|g_{k+1}\|^2} - (1 - \varpi_k) \frac{t \|y_k\|^2}{y_k^T s_k} \frac{(g_{k+1}^T s_k)^2}{y_k^T s_k \|g_{k+1}\|^2} \right]$$

since $g_{k+1}^T s_k \leq s_k^T y_k$

$$\frac{d_{k+1}^T g_{k+1}}{\|g_{k+1}\|^2} + 1 \leq \left[\frac{g_{k+1}^T y_k (s_k^T y_k)}{s_k^T y_k \|g_{k+1}\|^2} - t \varpi_k \frac{(s_k^T y_k)^2}{s_k^T y_k \|g_{k+1}\|^2} - (1 - \varpi_k) \frac{t \|y_k\|^2}{(s_k^T y_k)^2} \frac{(s_k^T y_k)^2}{\|g_{k+1}\|^2} \right]$$

$$y_k^T g_{k+1} \leq \|y_k\| \|g_{k+1}\|$$

$$\frac{d_{k+1}^T g_{k+1}}{\|g_{k+1}\|^2} + 1 \leq \frac{\|y_k\|}{\|g_{k+1}\|} = \mu, \text{ where } \mu > 0$$

$$\frac{d_{k+1}^T g_{k+1}}{\|g_{k+1}\|^2} + 1 \leq \mu$$

$$d_{k+1}^T g_{k+1} \leq -(1 - \mu) \|g_{k+1}\|^2$$

3.2. Global Convergent Properties

To prove the global convergence property, we need the relation $s_k^T y_k \geq m \|s_k\|^2, \forall x, y \in R^n, m > 0$ where m is constant, see [18-20]. The following assumption is needed in order to proceed with the proof of global convergence property.

Assumption 1

i) The level set $S = \{x : f(x) \leq f(x_0)\}$ is bounded, that is, there exists a constant $z > 0$, such $\|x\| \leq z, \forall x \in S$

ii) In neighborhood N of S , f is continuously differentiable, and its gradient is Lipschitz

$$\|g(x) - g(y)\| \leq L \|x - y\|, \quad \forall x, y \in N \quad (10)$$

Below the assumptions (i) and (ii) on f , we are able to deduce that there exists $\gamma > 0$ such as,

$$\gamma \leq \|\nabla f(x)\| \leq \bar{\gamma} \quad (11)$$

$$\text{iii) } (g(x) - g(y))(x - y) \geq \mu \|x - y\|^2, \quad \forall x, y \in S, \mu > 0 \quad (12)$$

Under this Assumption, the following lemma is obtained, which was proved by [11]

Lemma 1

Assume that Assumption-1 hold and suppose that for any CG-method d_{k+1} is a descent direction and the step size α_k is achieved by (7a,7b). If,

$$\sum_{k \geq 1} \frac{1}{\|d_{k+1}\|^2} = \infty \quad (13)$$

Then,

$$\liminf_{k \rightarrow \infty} \|g_k\| = 0 \quad (14)$$

Theorem 2

Suppose that Assumption-1 is true ,consider the new algorithm with β_k^{new} ,then the algorithm has

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

Proof:

$$\|d_{k+1}\| = \left\| -g_{k+1} + \left[\frac{g_{k+1}^T y_k}{y_k^T s_k} - \sigma_k \frac{g_{k+1}^T s_k}{y_k^T s_k} - (1 - \sigma_k) \frac{\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T s_k} \right] s_k \right\|$$

$$\|d_{k+1}\| \leq \|g_{k+1}\| + \left[\left| \frac{g_{k+1}^T y_k}{y_k^T s_k} \right| + |t\varpi_k| \left| \frac{g_{k+1}^T s_k}{y_k^T s_k} \right| + (1-\varpi_k) \left| \frac{t\|y_k\|^2}{y_k^T s_k} \frac{g_{k+1}^T s_k}{y_k^T s_k} \right| \right] \|s_k\|$$

Since $y_k^T g_{k+1} \leq \|y_k\| \|g_{k+1}\|$, $s_k^T g_{k+1} \leq s_k^T y_k$ and $s_k^T y_k \geq m\|s_k\|^2$

$$\|d_{k+1}\| \leq \|g_{k+1}\| + \left[\frac{\|g_{k+1}\| \|y_k\|}{m\|s_k\|^2} + |t\varpi_k| \frac{y_k^T s_k}{y_k^T s_k} + (1-\varpi_k) \frac{t\|y_k\|^2}{(y_k^T s_k)^2} \right] \|s_k\|$$

$$\|d_{k+1}\| \leq \|g_{k+1}\| + \left[\frac{\|g_{k+1}\| \|y_k\|}{m\|s_k\|^2} + |t\varpi_k| + (1-\varpi_k) \frac{t\|y_k\|^2}{m\|s_k\|^2} \right] \|s_k\|$$

Let
$$c_1 = \frac{\|g_{k+1}\| \|y_k\|}{m\|s_k\|^2} + |t\varpi_k| + (1-\varpi_k) \frac{t\|y_k\|^2}{m\|s_k\|^2}$$

$$\|d_{k+1}\| \leq \|g_{k+1}\| + c_1 \|s_k\| = \xi$$

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

4. DERIVATION OF THE MOFIFIED QN-METHOD

The purpose of this section is to create a new matrix which is a modified of memoryless BFGS method [21, 22]. Observe that the search directions, defined by (9) can be written by:

$$d_{k+1} = -Q_{k+1} g_{k+1}$$

where the matrix Q_{k+1} is given by:

$$Q_{k+1} = I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + t[\varpi_k + (1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k}] \frac{s_k s_k^T}{s_k^T y_k} \tag{15}$$

This matrix is considered as a modified memoryless BFGS method.

Lemma 2

If Q_1 is positive definite matrix then all matrix Q_{k+1} defined in (15) is also positive definite, i.e. $z_k^T Q_k z_k > 0$, for any vector $z \neq 0$.

Proof:

$$\begin{aligned} z_k^T Q_{k+1} z_k &= z_k^T \left[I - \frac{y_k s_k^T + s_k y_k^T}{s_k^T y_k} + t[\varpi_k + (1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k}] \frac{s_k s_k^T}{s_k^T y_k} \right] z_k \\ &= z_k^T z_k - \frac{(z_k^T y_k)(s_k^T z_k)}{s_k^T y_k} + \frac{(z_k^T s_k)(y_k^T z_k)}{s_k^T y_k} + t(\varpi_k + (1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k}) \frac{(z_k^T s_k)^2}{s_k^T y_k} \end{aligned}$$

$$= z_k^T z_k + \zeta_k, \text{ where } \zeta_k = t(\varpi_k + (1-\varpi_k)) \frac{\|y_k\|^2}{s_k^T y_k} \frac{(s_k^T z_k)^2}{s_k^T y_k}$$

Since $z_k^T z_k$, ζ_k are greater than zero. Then proof is complete.

Theorem 3

The matrix Q_{k+1} defined by (15) achieved the following QN-condition (i.e $Q_{k+1} y_k = \rho_k s_k$)

Proof:

Multiply (15) by y_k we get :

$$\begin{aligned} Q_{k+1} y_k &= \left[I - \frac{y_k s_k^T + s_k y_k^T}{s_k^T y_k} + t(\varpi_k + (1-\varpi_k)) \frac{\|y_k\|^2}{s_k^T y_k} \frac{s_k s_k^T}{s_k^T y_k} \right] y_k \\ &= y_k - \frac{y_k (s_k^T y_k)}{s_k^T y_k} - \frac{s_k (y_k^T y_k)}{s_k^T y_k} + t\varpi_k \frac{s_k (s_k^T y_k)}{s_k^T y_k} + t(1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k} \frac{s_k (s_k^T y_k)}{s_k^T y_k} \\ &= s_k \frac{\|y_k\|^2}{s_k^T y_k} + t\varpi_k s_k + t(1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k} s_k \\ &= \left[\frac{\|y_k\|^2}{s_k^T y_k} + t\varpi_k s_k + t(1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k} \right] s_k \end{aligned}$$

$$\text{Let } \left[\frac{\|y_k\|^2}{s_k^T y_k} + t\varpi_k s_k + t(1-\varpi_k) \frac{\|y_k\|^2}{s_k^T y_k} \right] = \rho_k$$

$$Q_{k+1} y_k = \rho_k s_k$$

5. RESULTS AND DISCUSSION

In this section we present the computational performance of a Fortran implementation of the HYBRID algorithm (New1) on a set of (750) unconstrained optimization test problems. The test problems are the unconstrained problems in the CUTE [7] library, along with other large-scale optimization problems presented in [23, 24]. We selected (75) large-scale unconstrained optimization problems in extended or generalized form. Each problem is tested (10) times for a gradually increasing number of variables: $n=1000, 2000, 10000$. To demonstrate the efficiency of the new algorithm, we used the Dolan and Moré method. The curve of the curve to the top indicates the new method better than the rest of the previous methods. All algorithms implement the Wolfe line search conditions with $\sigma = 0.9$ and $\delta = 0.001$ [25, 26], the same stopping criteria when $\|g_k\| \leq 10^{-5}$.

In the first set of numerical experiments we compare the new method with DL and HZ method. By calculating the number of the function evaluations (NOF), the frequency of the method (NOI) and the time required to implement the method (CPU), The new algorithm was compared to similar algorithms :

- A new proposed method (New) define by (8)
- DL conjugate gradient method define by (4)
- HZ conjugate gradient method (6)

Our demonstrated results are shown in Figures 1-6. We used the Dolan and Moré method [27, 28]. Figures 1-3, list the performance of the above methods relative to iterations number, the number of gradient evaluations and the CPU time, respectively. The second set of numerical experiments refers to the

comparisons of new method (15) with memoryless BFGS method. Figures 4-6, list the performance of the above methods. To demonstrate the efficiency of the new algorithm.

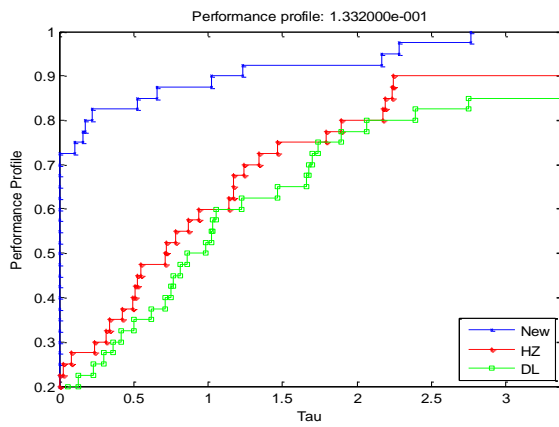


Figure 1. Performance profiles based on function evaluation

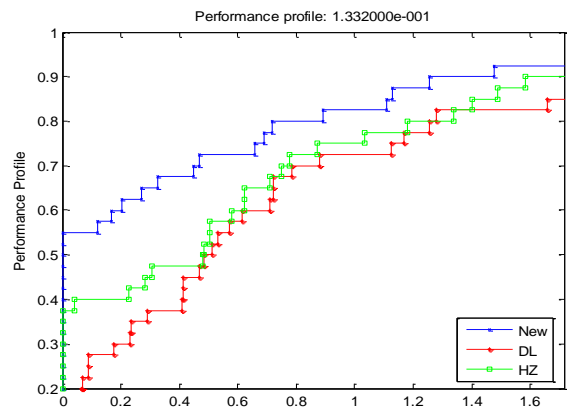


Figure 2. Performance profiles based on number of iterations

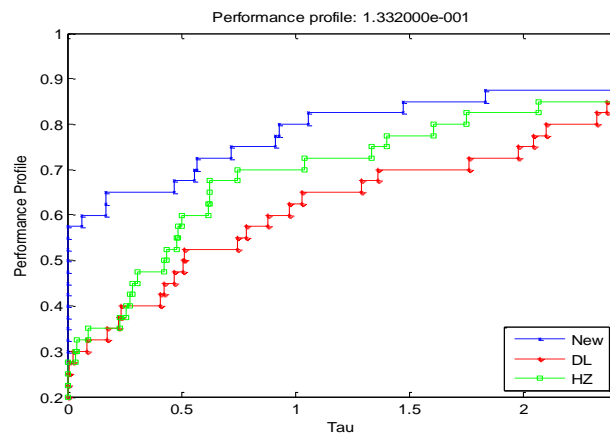


Figure3. Performance profiles based on CPU time

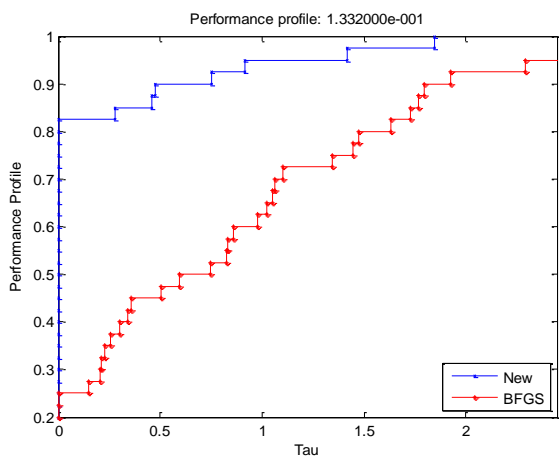


Figure 4. Performance profiles based on CPU time

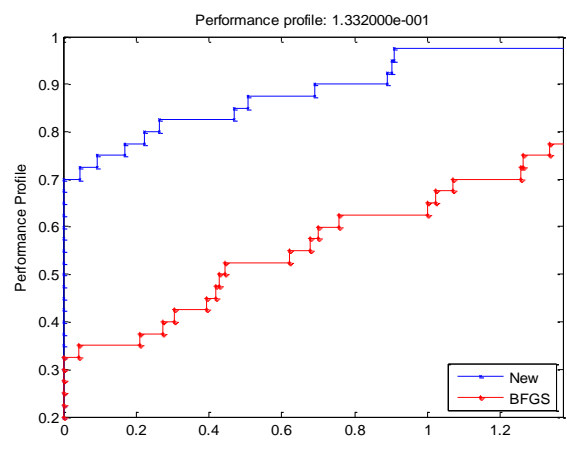


Figure 5. Performance profiles based on number of iterations

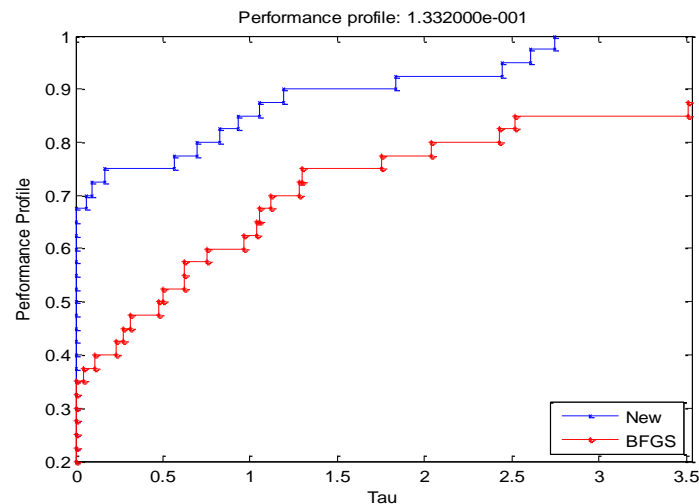


Figure 6. Performance profiles based on function evaluation

6. CONCLUSIONS

We suggested a linear combination between HZ and DL method and get a new proposed CG-method namely (2), (3) and (8) under some condition, we prove that our method is global convergent for convex functions. Also, we drive a new matrix defined in (15) and we have proved that its positive definiteness is achieved and satisfy the QN-condition. Numerical results showed that our suggested method gives an effective numerical result in practically.

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