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NUMERICAL AND CONVERGENCE ANALYSIS OF AN ENHANCED DAI-LIAO METHOD FOR UNCONSTRAINED OPTIMIZATION

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ABSTRACT

Iterative algorithms play an important role in mathematical optimization, particularly in solving large-scale unconstrained optimization problems. The conjugate gradient (CG) methods are widely used due to their low memory requirements and efficiency. However, their performance highly depends on the choice of parameters that influence search directions and convergence speed. Despite their advantages, traditional CG algorithms sometimes suffer from slow convergence or poor accuracy, especially for ill-conditioned problems. The selection of conjugate gradient parameters significantly influences the performance, and there is a need to develop improved strategies to enhance solution accuracy and efficiency. This study constructs a new conjugate gradient parameter using the curvature condition to refine search directions and accelerate convergence. The proposed approach ensures a more effective balance between descent properties and numerical stability. Preliminary numerical experiments demonstrate that the proposed method outperforms classical CG variants regarding convergence rate and accuracy. The improved search directions lead to faster and more reliable optimization solutions. The newly developed conjugate gradient formula contributes to a more robust and efficient optimization. This advancement enhances the applicability of CG methods in solving complex optimization problems, paving the way for more effective computational efficiency.

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1. INTRODUCTION

Large-scale unconstrained optimization lies at the core of numerous scientific and engineering challenges, including machine learning, motion control, computational physics, heat transfer, and resource allocation [1], [2], [3], [4], [5], [6], [7]. Recently, the demand for effective methods to solve such problems has grown exponentially, particularly with the continuous expansion of model complexities and datasets. Among iterative algorithms, nonlinear conjugate gradient (CG) formulas have emerged as crucial tools due to their simplicity, low memory requirements, and ability to avoid explicit computation of Hessian matrices [8], [9], [10]. Since their inception, CG formulas have evolved into a family of variants, including the Hestenes-Stiefel (HS) [11], Fletcher-Reeves (FR) [12], Polak-Ribière-Polyak (PRP) [13], [14], and Dai-Yuan (DY) [15], Conjugate Descent (CD) [16] methods. These algorithms iteratively refine search directions using parameters that balance descent properties and conjugacy conditions, enabling them to navigate high-dimensional spaces efficiently.

Despite their widespread adoption, classical CG algorithms are not without limitations. A critical challenge lies in the selection of the conjugate gradient parameter, β_k, which directly governs the search direction and, consequently, the algorithm's convergence behavior [9], [17]. Suboptimal choices of β_k can lead to inefficient step directions, resulting in slow convergence, stagnation, or even divergence, particularly for ill-conditioned or non-convex problems [18], [19]. For instance, the FR method may suffer from "jamming" phenomena, while the PRP method can lose global convergence guarantees under certain conditions [20]. Even modern hybrid approaches, such as the Dai-Liao (DL) method [21], which introduced a tunable parameter to unify classical formulas, face challenges in maintaining robustness across diverse problem landscapes [22]. This highlights the need for parameter selection strategies that better align with problem-specific curvature information and ensure a robust balance between descent properties and conjugacy requirements [23], [24].

Recent advancements have emphasized integrating curvature conditions into CG parameter design. The Dai-Liao method, for example, leverages the secant condition from quasi-Newton methods to enhance conjugacy [25], [26]. However, its performance remains sensitive to the choice of the tuning parameter t, which influences the trade-off between conjugacy and numerical stability [25]. Prior studies have demonstrated that improper parameterization can lead to insufficient descent or directional rigidity, limiting the method's applicability to complex optimization tasks [9], [25]. To address these gaps, this study proposes an enhanced Dai-Liao CG method that systematically incorporates curvature information through a novel parameterization strategy. By redefining β_k using a dynamically adjusted curvature-aware term, the proposed algorithm strengthens the conjugacy condition while preserving the global convergence properties essential for reliability.

The primary objectives of this research are as follows:

1. To derive a new β_k parameter that explicitly incorporates curvature information, ensuring stronger conjugacy and descent properties.
2. To establish rigorous global convergence guarantees under standard assumptions.
3. To validate the method's efficacy through comprehensive numerical comparisons against classical CG variants.

Theoretical analysis demonstrates that the proposed parameter satisfies the sufficient descent condition $g_k^T d_k \leq -c\|g_k\|^2$ and maintains bounded search directions, thereby enhancing numerical stability. Preliminary experiments on benchmark problems reveal significant improvements in convergence rates and solution accuracy, particularly for ill-conditioned and non-convex functions.

This study contributes to the broader topography of optimization by advancing the Dai-Liao structure, offering a more adaptable and robust CG algorithm. The improved conjugate gradient method bridges the gap between theoretical conjugacy requirements and practical numerical performance. It is a viable candidate for high-dimensional optimization applications like deep learning and large-scale simulations. By addressing the limitations of traditional parameter selection strategies, this research paves the way for more efficient and reliable computational tools in data-driven domains.

2. RESEARCH METHOD

The conjugate gradient formula is designed to tackle the optimization problem of the form:

$$Minf(x) \ , \ x \in R^n \tag{1}$$

where f is a smooth function [27]. The CG algorithm usually generates a sequence of iterates using the following recursive formula:

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

where α_k is the step-size and d_k is the search-direction, which is defined as follows [28]:

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

2.1 Related Work

In the conjugate gradient direction **Equation (3)**, β_k is a parameter that defines characterize different CG methods. Some of the classical techniques mentioned above have the following formulas:

$$\begin{aligned} \beta_k^{FR} &= \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \\ \beta_k^{PRP} &= \frac{y_k^T g_{k+1}}{g_k^T g_k} \\ \beta_k^{HS} &= \frac{g_k^T y_k}{d_{k-1}^T y_{k-1}} \\ \beta_k^{DY} &= \frac{g_{k+1}^T g_{k+1}}{y_k^T s_k} \\ \beta_k^{CD} &= \frac{g_k^T g_k}{d_{k-1}^T g_{k-1}} \end{aligned} \tag{4}$$

Each of the above formulas has its unique strengths. For instance, the FR method ensures global convergence, while the PRP formula often performs better in practice. HS algorithm is direction-sensitive, CD maintains conjugacy through gradient projection, while DY is conservative but globally convergent [9].

To meet specific requirements, step length α_k is often selected in iterative approaches. The following criteria must be satisfied in order for the Wolfe conditions to be used in convergence analysis and conjugate gradient technique implementations:

$$f(u_k + \alpha_k d_k) \leq f(u_k) + \delta . \alpha_k g_k^T d_k \tag{5}$$

$$d_k^T g(u_k + \alpha_k d_k) \geq \sigma . d_k^T g_k \tag{6}$$

where $0 < \delta < \sigma < 1$ [29]. Regretfully, if the objective function is nonconvex and the usual Wolfe line search is applied, all of the presented techniques might not converge.

The theoretical advantages and computational advantages of the conjugate gradient methods proposed by Dai-Liao in [21] were attempted to be attained once again, as:

$$\beta_k^{DL} = \frac{g_{k+1}^T y_k - t g_{k+1}^T s_k}{d_k^T y_k} \tag{7}$$

An extra effort was placed into achieving the computational and theoretical benefits of the conjugate gradient approaches (see; [8], [30], [31], [32]).

It is captivating to employ the conjugate gradient method within mathematical constructs. An innovative equation that conforms to the curvature criterion is developed. In contrast to the Dai-Liao paradigm, which amalgamates gradient and differential point information in its computations, the refined

technique exhibits enhanced efficiency by utilizing functional data. Empirical numerical analyses are performed to demonstrate the effectiveness of the recently introduced methodology.

2.2 New Method Formulation

Based on quadratic model, Basim et al. [30] presented a curvature condition which is written explicitly as:

$$s_k^T Q(u_k) s_k = (f_k - f_{k+1}) + 1/2 s_k^T y_k \tag{8}$$

By inserting $B_{k+1} \cong Q(u_k)$ into **Equation (8)** we conclude that:

$$s_k^T B_{k+1} s_k \cong (f_k - f_{k+1}) + 1/2 s_k^T y_k \tag{9}$$

Inside [33], Perry's conjugacy condition as ($d_{k+1}^T y_k = -g_{k+1}^T s_k$) and using in the **Equation (9)**, it is obtained:

$$d_{k+1}^T B_{k+1} s_k \cong -\left[1/2 + (f_k - f_{k+1})/s_k^T y_k\right] g_{k+1}^T s_k \tag{10}$$

Therefore, it can be seen that:

$$d_{k+1}^T B_{k+1} s_k \cong -(1/2 + (f_k - f_{k+1})/s_k^T y_k) g_{k+1}^T s_k \tag{11}$$

Hence, by **Equation (11)** and search direction d_{k+1}, we have:

$$(-g_{k+1} + \beta_k d_k)^T y_k \cong -(1/2 + (f_k - f_{k+1})/s_k^T y_k) g_{k+1}^T s_k \tag{12}$$

This implies:

$$\beta_k^{Dai-Liao\ (BC)} = \frac{g_{k+1}^T y_k - \left[1/2 + (f_k - f_{k+1})/s_k^T y_k\right] g_{k+1}^T s_k}{s_k^T y_k} \tag{13}$$

They are referred to as Dai-Liao (BC) for convenience.

Algorithm 1. Dai-Liao (BC).

Input: Minimize a nonlinear function, edit $\boldsymbol{x_0} \in \boldsymbol{R^n}$, $\boldsymbol{\varepsilon}$.

Output: Minimizer x such that gradient is approximately zero.

1. If $\|\boldsymbol{g_k}\| < \boldsymbol{\varepsilon}$ stop.
2. Obtain $\boldsymbol{\alpha_k}$ by **Equation (5)** and **Equation (6)**.
3. Update $\boldsymbol{x_{k+1}} = \boldsymbol{x_k} + \boldsymbol{\alpha_k d_k}$ and $\boldsymbol{\beta_k}$ by **Equation (14)**.
4. Compute $\boldsymbol{d_{k+1}} = -\boldsymbol{g_{k+1}} + \boldsymbol{\beta_k s_k}$.
5. Set $\boldsymbol{k} = \boldsymbol{k} + \boldsymbol{1}$ and return to step 2.

3. RESULTS AND DISCUSSION

3.1 Convergence Results

The global convergence theorem of Algorithm Dai-Liao (BC) is proved using the following presumptions:

Assumption 3.1

1. Level is set to $L_0 = \{x \in R^n : f(x) \leq f(x_0)\}$ be convex.
2. Since the gradient is Lipschitz continuous, a positive constant is present $L > 0$:

$$\left(\nabla f(\bar{o}) - \nabla f(v^{+})\right) \leq L\left\|\bar{o} - v^{+}\right\| \ , \forall \bar{o}, v^{+} \in L_0. \tag{14}$$

3. Assumptions 1 and 2 immediately imply that there is a positive constant $\Pi > 0$ such that:

$$\|g_{k+1}\| \leq \Pi. \tag{15}$$

Theorem 1. *Let* $\boldsymbol{d_{k+1}}$ *be generated based on Dai-Liao (BC) formula framework. Then:*

$$d_{k+1}^{T} g_{k+1} \leq 0 \tag{16}$$

Proof:

Using **Equation (4)** is definition of d_{k+1}, we obtain:

$$d_{k+1}^{T} g_{k+1} = -\|g_{k+1}\|^2 + \left(\frac{g_{k+1}^{T} y_k - \left[1/2 + (f_k - f_{k+1})/s_k^{T} y_k\right] g_{k+1}^{T} s_k}{s_k^{T} y_k}\right) s_k^{T} g_{k+1} \tag{17}$$

By using Lipschitz continuity, we obtain:

$$g_{k+1}^{T} y_k \leq L g_{k+1}^{T} s_k \tag{18}$$

When we entered **Equation (18)** into **Equation (17)**, we got:

$$d_{k+1}^{T} g_{k+1} = -\|g_{k+1}\|^2 + [L-1]\frac{(s_k^{T} g_{k+1})^2}{s_k^{T} y_k} \tag{19}$$

From the inequality above, we obtain:

$$\begin{aligned} d_{k+1}^{T} g_{k+1} &\leq -\|g_{k+1}\|^2 - [1-L]\frac{(s_k^{T} g_{k+1})^2}{s_k^{T} y_k} \\ &\leq -\|g_{k+1}\|^2 < 0 \end{aligned} \tag{20}$$

The proof is ended. ■

Zoutendijk published this conclusion, which is crucial to understanding CG formula **[33]** .

Lemma 1. *Assume that the direction produced by* ***Equation (4)*** *and is correct. If:*

$$\sum_{k\geq 0} \frac{1}{\left\|d_{k+1}\right\|^2} = \infty \ , \tag{21}$$

Then:

$$\lim_{k\to\infty} \inf \ \left\|g_{k+1}\right\| = 0 \tag{22}$$

Theorem 2. *Let f is uniformly convex on* $\boldsymbol{\tau}$*, explicitly, there exist a constant* $\boldsymbol{\Phi > 0}$ *as:*

$$\left(\nabla f(x) - \nabla f(y)\right)^{T}\left(x - y\right) \geq \Phi\left\|x - y\right\|^2 \quad \forall \ x, y \in \tau \ . \tag{23}$$

If $\{x_k\}$ is obtained by new Algorithm, then:

$$\lim_{k\to\infty} \inf \ \left\|g_{k+1}\right\| = 0 \tag{24}$$

.

Proof.

From the new $\beta_k^{\text{Dai-Liao (BC)}}$, we get:

$$\beta_k^{\text{Dai-Liao (BC)}} \leq \frac{|g_{k+1}^{T} y_k| + |g_{k+1}^{T} s_k|}{|s_k^{T} y_k|}. \tag{25}$$

By **Equation (25)** and **Equation (23)**, we obtain:

$$\beta_k^{BBX} \leq \frac{\Pi L\|s_k\| + \Pi\|s_k\|}{\Phi\|s_k\|^2} \tag{26}$$

Substituting **Equation (28)** into **Equation (4)** give:

$$\begin{aligned} \|d_{k+1}\| &= \left\|-g_{k+1} + \beta_k^{\text{Dai-Liao (BC)}} d_k\right\| \\ &\leq \Pi + \frac{\Pi L\|s_k\| + \Pi\|s_k\|}{\Phi\|s_k\|^2}\|s_k\| \\ &\leq C\Pi. \end{aligned} \tag{27}$$

where $C = 1 + (L+1)/\Phi$. As a result, we obtain that:

$$\sum_{k\geq 1}\frac{1}{\|d_{k+1}\|^2} \geq \frac{1}{C\Pi}\sum_{k\geq 1} 1 = \infty \tag{28}$$

from **Lemma 1**, implies that $\lim_{k\to\infty} inf\|g_k\| = 0$.

3.2. Numerical Results

This section presents a comprehensive evaluation of the proposed method's computational efficiency compared to the classical Hestenes-Stiefel (HS) method as described in [34]. The numerical experiments were conducted using a set of standard unconstrained optimization test problems taken from the collection proposed by Andrei [34], with problem dimensions varying between 100 and 1000.

Table 1. Table of problems, Starting Points and Dimensions.

Problem	Dim	Function No.	starting points
Freudnstein & Roth	100, 1000	1, 2	$x_0 = [0.5, -2, 0.5, -2, \ldots\ldots, 0.5, -2]$
Trigonometric	100, 1000	3, 4	$x_0 = [0.2, 0.2, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 0.2]$
Pertorbed Quadrtic	100, 1000	5, 6	$x_0 = [0.5, 0.5, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 0.5]$
Extended Tridiagonl 1	100, 1000	7, 8	$x_0 = [2, 2, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 2]$
Exteded Three Expo Terms	100, 1000	9, 10	$x_0 = [0.1, 0.1, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 0.1]$
Genzralized Tridagonal 2	100, 1000	11, 12	$x_0 = [-1, -1, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, -1]$
Exteded PSC1	100, 1000	13, 14	$x_0 = [3, 1, 3, 1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 3, 1]$
Extended-Powell	100, 1000	15, 16	$x_0 = [3, -1, 0, 1 \ldots\ldots\ldots\ldots\ldots\ldots 1, 0, 1]$
Extanded-Cliff	100, 1000	17, 18	$x_0 = [0, -1, 0, -1 \ldots\ldots\ldots\ldots\ldots, 0. -1]$
Quadrtic Digonal	100, 1000	19, 20	$x_0 = [0.5, 0.5, \ldots\ldots\ldots\ldots\ldots, 0.5]$
Extended-Hiebert	100, 1000	21, 22	$x_0 = [0, 0, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 0]$
QP2	100, 1000	23, 24	$x_0 = [0.5, 0.5, \ldots\ldots\ldots\ldots\ldots\ldots, 0.5]$
.NONDIA (CUTE)	100, 1000	25, 26	$x_0 = [1.0, 1.0, \ldots\ldots\ldots\ldots\ldots\ldots 1.0]$
.DIXMAANE (CUTE)	100, 1000	27, 28	$x_0 = [2, 2, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, 2]$
Almost Pertubed	100, 1000	29, 30	$x_0 = [0.5, 0.5, \ldots\ldots\ldots\ldots\ldots\ldots, 0.5]$

To assess the performance of both methods, three key performance indicators were used: the number of iterations (NI) required for convergence, the number of restarts (NR) triggered during the optimization process, and the number of function evaluations (NF) performed. These metrics provide a holistic view of the computational cost and robustness of the methods under study.

All numerical experiments were executed using the well-established Wolfe line search strategy. The parameters for the Wolfe conditions were set to $\delta = 0.001$ and $\sigma = 0.9$, ensuring a balance between sufficient decrease and curvature conditions during the line search process. The stopping criterion for the optimization was defined as $\|g_{k+1}\| \leq 10^{-6}$, where g_{k+1} denotes the gradient at the (x_{k+1})-th iteration.

Table 2 below summarizes the list of test problems selected for the evaluation and presents the corresponding numerical results, highlighting the comparative performance of the proposed method against the classical HS algorithm.

Table 2. Table of Number of Iterations, Number of Restarts and Function Evaluations

		HS			Dai-Liao (BC)		
Problem	**Dim**	**NI**	**NR**	**NF**	**NI**	**NR**	**NF**
1	100	102	95	2709	12	7	28
2	1000	14	8	32	12	7	28
3	100	19	10	35	18	9	34
4	1000	39	22	67	35	21	62
5	100	102	33	155	84	23	128
6	1000	352	100	543	329	86	512
7	100	10	5	21	7	4	15
8	1000	14	7	27	13	7	26
9	100	13	8	23	10	6	16
10	1000	52	45	1225	42	38	934
11	100	42	17	62	37	14	59
12	1000	67	26	102	63	24	98
13	100	8	6	17	8	6	17
14	1000	26	25	505	7	5	15
15	100	79	19	149	73	24	142
16	1000	75	20	143	74	22	143
17	100	9	7	23	12	9	31
18	1000	37	35	844	12	9	28
19	100	46	7	82	56	8	101
20	1000	182	35	320	156	28	273
21	100	83	52	182	79	50	174
22	1000	79	50	171	79	50	171
23	100	23	12	543	24	13	56
24	1000	35	20	85	35	20	85
25	100	13	7	26	15	8	30
26	1000	15	8	31	15	8	31
27	100	81	28	126	70	23	113
28	1000	243	70	383	230	71	357
29	100	104	33	157	94	27	142
30	1000	330	96	516	302	83	470
Total		**2294**	**906**	**9304**	**2003**	**710**	**4319**

The above results were further analyzed using a performance profile tool introduced by Dolan and More **[35]**. This tool is a cumulative distribution function that represents the probability that a given method will solve a problem within a multiple of the best observed performance. The -axis from the plotted curve defines the performance ratio, while the -axis denotes the fraction of test problems solved within that ratio. Any algorithm whose curve lies on top of other curves is regarded as the better method, indicating the algorithm solves a larger proportion of functions more efficient.

Figure 1 illustrates the proposed algorithm's performance profile curve compared to the classical HS algorithm based on NI to show how quickly each algorithm converges. The curve shows that the proposed Dai-Liao (BC) method outperformed the classical HS algorithm because it attained a faster cumulative performance. This indicates that the proposed algorithm requires fewer iterations to attain convergence on

most test functions. The classical HS curve lags, indicating that it generally requires more iterations, which can impact computational efficiency.

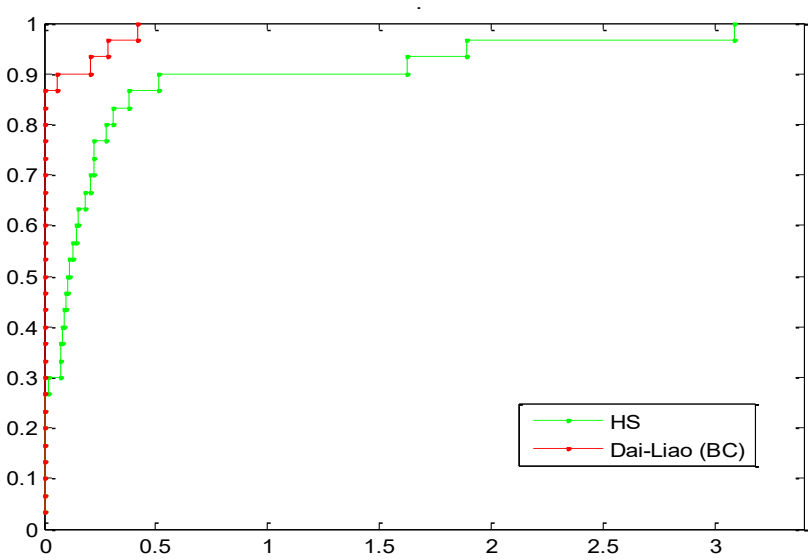

Figure 1. Performance on the Number of Iterations

Similarly, by assessing the second performance curve, which evaluated the number of restarts required for convergence, the proposed algorithm further shows superior performance, solving a higher proportion of problems with fewer restarts. The results implied that the classical HS algorithm takes longer to reach the same cumulative fraction of solved functions, suggesting that it may experience more difficulties maintaining stable convergence and requires more frequent restarts.

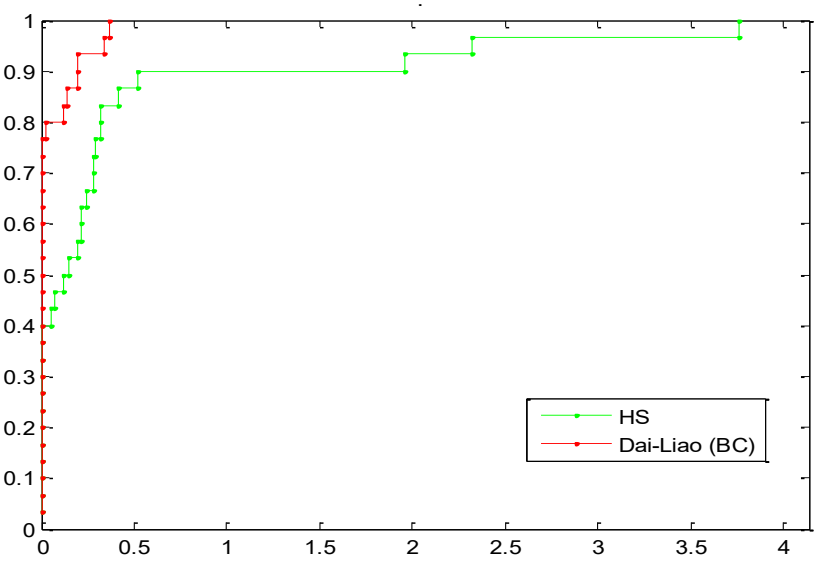

Figure 2. Performance on the Number of Restarts

Lastly, the results for function evaluations as displayed in **Figure 3** demonstrated that it directly impacts the computational cost of an optimization algorithm. However, the curve further confirms the efficiency of the proposed algorithm as its curve (the red line) dominates the green line, indicating that proposed algorithm consistently requires fewer function evaluations to reach an optimal solution. Since function evaluations are often the most expensive part of an optimization process, this result highlights the computational advantage of the proposed Dai-Liao (BC) over the classical HS algorithm.

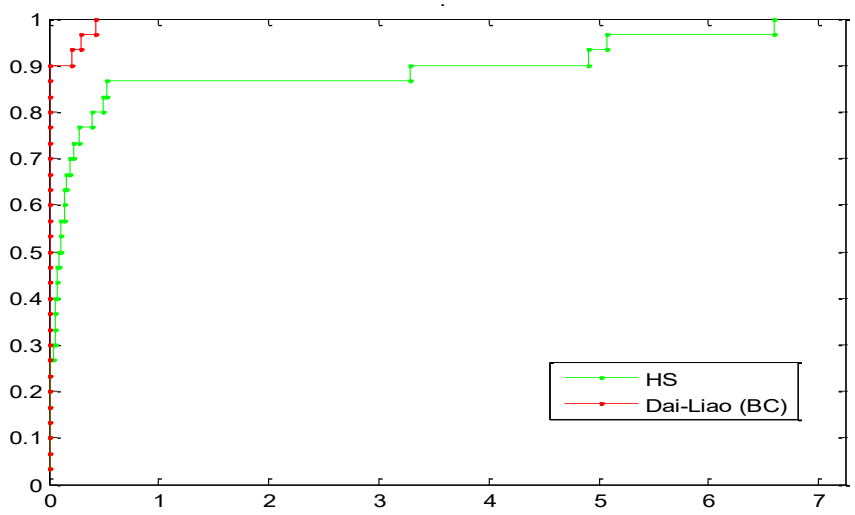

Figure 3. Function Evaluations Performance

These results support the selection of the proposed Dai-Liao (BC) for practical optimization problems where efficiency is a priority.

4. CONCLUSION

This study proposed a new conjugate gradient formula for unconstrained application optimization problems. The study established the proposed method's convergence under suitable conditions and showed that the direction is a descent direction. The numerical performance of the proposed methods was compared with the classical HS method based on three key metrics: the number of iterations, the number of restarts, and function evaluations. Findings from the numerical experiment show that our proposed Dai-Liao (BC) approach, designed based on curvature conditions, exhibits competitive performance and offers significant improvements in all the metrics, including the number of iterations, the number of restarts, and function evaluations, making it a viable alternative for solving unconstrained optimization problems.

AUTHOR CONTRIBUTIONS

Basim A. Hassan: Conceptualization, Writing – review, Formal analysis, Methodology. Ibrahim Mohammed Sulaiman: Writing - original draft, Validation, Resources. Yeldez J. Subhi: Software, Supervision, Visualization. All authors discussed the results and contributed to the final manuscript.

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CONFLICT OF INTEREST

The authors declare that no conflicts of interest exist in the study.

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