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A Scaled Nonlinear Conjugate Gradient Method for Unrestricted Optimizations

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Abstract: The conjugate gradient (CG) methods are a family of iterative algorithms used to repeatedly (or iteratively) solve nonlinear systems and control theory problems that can be formulated as unconstrained optimisation. The conjugate gradient method is used for some algorithms; a subclass of it is the hybrid conjugate gradient method. This paper provides new spectral and hybrid conjugate gradient methods. The innovative spectral conjugate gradient technique demonstrates global convergence features, supported by many presumptions and a rigorous Wolfe line search. Moreover, the hybrid conjugate gradient technique fulfils the requirements for achieving global convergence when employing accurate line searches. Additionally, we demonstrate that the approaches provided in this study meet the necessary conditions for descent. The suggested solutions exhibit a high level of competitiveness and efficiency, as evidenced by the numerical results obtained from several test problems.

Keywords: *conjugate gradient approach; spectral conjugate gradient; global convergence analysis; Wolfe line condition.*

Mathematics Subject Classification (2020): 90-XX, 93-XX, 90C06, 70Kxx.

1 Introduction

In numerous nonlinear dynamic systems, the objective is to determine the best state or combination of parameters that leads to the desired behavior. Optimizing parameters in control systems is frequently required to ensure stability and prevent oscillations. Gradient methods can also be applied to address nonlinear systems that arise from electronic and electrical circuits. Hence, the difficulty arising from the concerns mentioned above

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can be framed as an optimization problem, and an attempt can be made to resolve it using iterative techniques such as the way suggested in this paper, see [1, 2].

Consider the following problem with unconstrained optimization:

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

Let $f : \mathbb{R}^{\ltimes} \to \mathbb{R}$, if we think intuitively in terms of the graph of f, then we have a gradient map $(\nabla f)(x)$ mapping smoothly on the set R. In mathematics, we have 3 types of solutions exact, approximate and numeric methods. Numerical methods to solve Eq. (1) are a lot of them. Newton technique, conjugate gradient (CG), steepest descent(SD), and quasi-Newton(QN) methods belong to these types two. This means that for huge problems where the conjugate gradient method is not only extremely simple but also takes much less memory. Conjugate gradient method is quite efficient. Conjugate gradient methods enabled the numerical type classification. The bracketing method begins with an initial guess x^0 and then provides new guesses which converge to a solution of Eq. (1) by repetitively enhancing the bound via an iteration x^n. From here we are going to compute our target function f(x) for the first object and then calculate it for the other iterations x^1, x^2, x^3, x^4 and so on. Typically, in a non-linear conjugate gradient procedure, it is an iterative approach to solve for the optimal solution.

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

The step-length α_k is usually determined by means of one of the line searches. A Wolfe, Goldstein or Armijo criterion provides a proper step of $x^(k)$ so as to calculate some decrease in the function value without taking small steps. The first two terms guarantee that the attention flows in the direction p^k is given by

$$p_{k+1} = \begin{cases} -g_{k+1} & if \quad k=0, \\ -g_{k+1}+\beta_k p_k & if \quad k>0. \end{cases} \tag{3}$$

Within the framework of a three-term conjugate gradient approach (TTCG), as elucidated by N. Andrei [2], it is possible to choose from various generic formats

$$p_{k+1} = \begin{cases} -g_{k+1} & if \quad k=0, \\ -g_{k+1}-\alpha s_k - b y_k & if \quad k>0. \end{cases} \tag{4}$$

A search direction is determined by adding the values of g_{k+1}, s_k, y_k, when α_k and b_k implemented the mathematical formula associated with the terms $||g_k||^2, ||g_{k+1}||^2, ||y_k||^2, s_k^T g_k$ and $y_k^T\ g_k$, etc. $a_k = \beta_k$ is a commonality. Here, β_k is a parameter $(0 < \beta_k < 1)$ and g_{k+1} represents $g(x_{k+1})$. There are a number of formulas for β_k, which are listed below.

In this context, where $|.|$ is the Euclidean norm, $g_{k+1} = g(x_{k+1})$ and $y_k = \bigtriangledown f_{k+1} - \bigtriangledown f_k$ are vectors. We should be sure that function value is transported down as expected and there are not many iterations. These criteria, including Wolfe and Goldstein, Armijo conditions that are widely used to compute the step length α^k actually. The line search (LS) process is usually addressed with an inexact line search (ILS), like the Strong Wolfe Conditions (SWC) that help also define which $alphak$ assumes the statement above when conducting the theoretical convergence analysis of CG method. [7],

$$f(x_k+\alpha_k d_k) \le f(x_k)+\delta\alpha_k g_k^T p_k,\ 0 \le \delta \le \frac{1}{2}|p_k^T g(x_k+\alpha_k d_k)| \le -\sigma p_k^T g_k\ , \delta \le \sigma \le 1. \tag{5}$$

$\beta_k^{FR} = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k}$ [3]	$\beta_k^{CD} = \frac{g_{k+1}^T g_{k+1}}{-p_k^T g_k}$ [4]	$\beta_k^{BA1} = \frac{y_k^T y_k}{-p_k^T g_k}$ [10]
$\beta_k^{HS} = \frac{g_{k+1}^T y_{k+1}}{d_k^T y_k}$ [2]	$\beta_k^{LS} = \frac{g_{k+1}^T g_{k+1}}{-p_k^T g_k}$ [2]	$\beta_k^{BA2} = \frac{y_{k+1}^T y_{k+1}}{g_k^T g_k}$ [10]
$\beta_k^{PR} = \frac{g_{k+1}^T y_{k+1}}{g_k^T g_k}$ [7]	$\beta_k^{DY} = \frac{g_{k+1}^T g_{k+1}}{p_k^T y_k}$ [8]	$\beta_k^{BA3} = \frac{y_{k+1}^T y_{k+1}}{p_k^T y_k}$ [10]

Table 1: Classical Conjugate Gradient Conjugacy Parameters.

Recently, some scholars have presented innovative strategies and revised procedures, as evidenced in references [9–17]. In the subsequent sections, we will examine the given formula in detail, prove its attribute of decreasing, and offer valuable insights into its convergence.

2 New Direction for CG

Recent research has focused on enhancing the standard conjugate gradient approach by consolidating parameters inside the conjugate gradient methodology. Various hybrid algorithms were developed to use the strengths of classical conjugate gradient algorithms. Numerous hybrid methods were explored with the aim of obtaining conjugate gradient methods that were computationally efficient and exhibited favourable convergence features. Hybrid CG outperforms standard conjugated gradient algorithms [18, 19]. Malik *et al.* [20] have just created a novel β_k which is derived from the formula β_k^{NPRP}. The coefficient β_k is defined in the following manner:

$$\beta_k^{NPRP} = \begin{cases} X, & if \quad Y \\ 0 & otherwise, \end{cases} \tag{6}$$

where

$$X = \frac{||g_k||^2 - \frac{||g_{k+1}||}{||g_k||}|g_{k+1}^T g_k| - |g_{k+1}^T g_k|}{||p_{k+1}||^2}, \tag{7}$$

$$Y = ||g_{k+1}||^2 > \left(\frac{g_{k+1}}{g_k} + 1\right) |g_{k+1}^T g_k|. \tag{8}$$

Using an equation similar to the one described above, we propose our approach which incorporates new computed values of β_k along with another spectral parameter θ_k. In Eq.(6), we integrate an X -equation into the modification of Eq. (7).

$$\beta_k^{NPRP} = \begin{cases} X, & if \quad Y \\ 0 & otherwise, \end{cases} \tag{9}$$

$$X = \beta_k^{BA}. \tag{10}$$

β_k^{BA2}, as mentioned in Table 1 for Al-Bayati and Al-Asaady and $Y = ||g_{k+1}||^2 > \omega_k, |g_{k+1}^T g_k|, \omega_k = \frac{||g_{k+1}||}{||g_k||} + 1$, stay with the switch criteria. The imbalance of the formula BA2 is because the amount in the numerator is y^T y, it is the same problem found as in the Polak-Ribiere formula for conjugacy, where the method is frequently recovered when the slope in the new step is less than the old one. Also, frequent retrieval causes the conjugacy parameter to become zero, slowing down the regression. Therefore, the return had to be done carefully and with the scale set below for that purpose. Furthermore, it is possible that the spectral search direction facilitates the rapid descent towards the optimal point. The main difference between standard and spectral conjugate gradient methods is the computation of the search direction P_k. The search direction of the normal conjugate gradient method is determined by applying the formula Eq. 3, but the search direction of the spectral conjugate gradient method is determined by scaling g_k using the formula

$$p_{k+1} = \begin{cases} -g_{k+1} & if\ k=0, \\ -\theta_k g_{k+1} + \beta_k p_k, & if\ k>0. \end{cases} \tag{11}$$

In addition, Zhang et al. [21] also proposed a spectral conjugate gradient method which is called the SCD method. The SCD method is applied based on conjugate gradient coefficient (β_k) and spectral gradient parameter (θ_k):

$$\beta = \beta_k^{FR}\ and\ \theta_k = \frac{p_k^T y_k}{||g_k||^2}. \tag{12}$$

The conjugacy parameter (β^{MAR}) is imported and positioned in the second term of Eq.(6). The trend's ultimate manifestation is defined by newly established parameters:

$$\beta_k^{NPRP} = \begin{cases} X, & if \quad Y \\ 0 & otherwise, \end{cases} \tag{13}$$

$$X = \beta_k^{NPRP}\ and\ Y = ||g_{k+1}||^2 > \omega_k, |g_{k+1}^T g_k|, \omega_k = \frac{||g_{k+1}||}{||g_k||} + 1. \tag{14}$$

Denote the conjugate parameter β_k^{NPRP} and spectral scaling for the gradient θ_k^{NPRP} as follows:

$$\theta_k = \frac{p_k^T y_k}{||g_k||^2}. \tag{15}$$

2.1 MAR-CG algorithm

Process (0): initialization, as start $k = 0$, set: $x_0 \epsilon \mathbb{R}^n$, compute all $f(x_0)$, $g(x_0)$, let $p_0 = -g_0$ and $\alpha_0 = 1/||g_0||_2$.
Process (1): Check for convergence: If $\|g_k\| \leq \epsilon$, then stop; x_k is the optimal solution; Else continue with Process (2).
Process (2): Second, obtain α_k in the line search process bearing in mind the Wolfe conditions and set variable $x_{k+1} = x_k + \alpha_k p_k$. Now coming to the input, find out f_{k+1}, g_{k+1}, y_k and p_k.
Process (3): Obtain the direction defined by $p_= - \theta_k^{MAR} g_{k+1} + \beta_k^{MAR} p_k$, β_k^{MAR} is set as described in Eq. (13).
Process (4): If we are satisfied with restarts from Powell's, set $p_{k+1} = -g_{k+1}$ and if not, set $p_{k+1} = p$.
Process (5): If we are satisfied with restarts from Powell's, set ($p_{k+1} = -g_{k+1}$) and if not set ($p_{k+1} = p$)
Process (6): Initialize the estimate with $\alpha_k = \alpha_{k-1}\left(\frac{||p_k||_2}{||pk-1||_2}\right)$, set $k = k+1$ and go back to Process (1).

3 Analysis of Convergence

We need to show that the new CG-Algorithms are globally convergent, which is a necessary condition.

3.1 Assumptions (H):

(i) We know that the set: $s = \{x : x \in R_n, f(x) \leq f(x_1)\}$ is bounded. Here, x_1 is the starting point and $c > 0$ is a constant. The following statement is true for all $B > 0$.
(ii) The model f is continuously-differentiable in the neighborhood Ω of S, and the gradient g satisfies a Lipschitz condition. Let $L \geq 0$ be a constant such that

$$||g(x) - g(y)|| \leq L||x - y|| \ \forall\, x, y\epsilon\Omega. \tag{16}$$

Now, by Assumption (H)(i), we can clearly find a positive constant D such that

$$B = max||x - y||, \ \forall\, x, y\epsilon S. \tag{17}$$

Define the set B to be the diameter of the domain Ω. From (H)(ii) we can actually deduce that there exists a positive constant $\Upsilon \geq 0$ such that:

$$||g(x)|| \leq \Upsilon, \ \forall\, x\epsilon S. \tag{18}$$

However this correct descent or descent condition is statistically problematic to ensure in general (see [3] for computational based methods in particular).

3.2 Theorem (Descendant property):

For simplicity, let us assume that Assumptions (H) are satisfied and that we use a line search method with strong Wolfe conditions as discussed in Sec. We prove in Eqs. (5) that the search directions p_k *can be obtained from them. In (14) and (15),* $c = \frac{(p_k^T y_k)}{||g_k||^2}$ *immediately satisfies the required steering search sufficient condition;*
$p_{k+1}^T g_{k+1} \leq -c||g_{k+1}||^2$.

Proof. Start with multiplying the direction p_{k+1} in Eq. (14) by the gradient g= g_{k+1},

$$p_{k+1}^T g = -\theta_k^|\,|g||^2 + \beta_k^{MAR} p_k^T g. \tag{19}$$

We have the condition $||g_{k+1}||^2 > \omega_k |g_{k+1}^T g_k|$ to switch between $\beta_k^{MAR} = 0$ or β_k^{BA}. In this case, $\beta_{k+1}^{MAR} = 0$ makes the descent hold directly.
Otherwise, set the value of the parameters β_k^{MAR} and θ_k,

$$p_{k+1}^T g_{k+1} = -\frac{p_k^T y_k}{||g_k||^2}||g_{k+1}||^2 + \frac{y_k^T y_k}{||g_k||^2} p_k^T g_{k+1}.$$

Utilize the reality given from the strong Wolfe conditions $p_k^T\ g_{k+1} < p_k^T\ y_k$, we get the inequality

$$p_{k+1}^T g_{k+1} \leq -\frac{p_k^T y_k}{||g_k||^2}||g_{k+1}||^2 + \frac{y_k^T y_k}{||g_k||^2} p_k^T y_k.$$

Or, we can rearrange the last term

$$p_{k+1}^T g_{k+1} \leq -\frac{p_k^T y_k}{||g_k||^2}||g_{k+1}||^2 + \frac{y_k^T y_k}{||g_k||^2} y_k^T y_k.$$

We have $y_k^T y_k = ||g_{k+1}||^2 + ||g_k||^2 - 2g_{k+1}^T g_k$, it implies that

$$p_{k+1}^T g_{k+1} \leq -\frac{(p_k^T y_k)}{||g_k||^2}||g_{k+1}||^2 + \frac{p_k^T y_k)}{||g_k||^2}(||g_{k+1}||^2 + ||g_k||^2 - 2g_{k+1}^T g_k)$$

$$p_{k+1}^T g_{k+1} \leq \frac{p_k^T y_k}{{g_k}^2}(||g_k||^2 - 2g_{k+1}^T g_k)$$

and A^T B$\leq \frac{1}{2}(A^2 + B^2)$ helps as in the second term

$$p_{k+1}^T g_{k+1} \leq \frac{p_k^T y_k}{||g_k||^2}||g_k||^2 - 2\frac{p_k^T y_k}{2{g_k}^2}(||g_{k+1}||^2 + ||g_k||^2)$$

$$p_{k+1}^T g_{k+1} \leq -c||g_{k+1}||^2$$

with c $= \frac{p_k^T y_k}{{g_k}^2}$.

3.3 Property (Boundedness of β_k)

Let us consider the existence of a generic conjugate gradient method and assume that [21]

$$\zeta \leq ||g_k|| \leq \Upsilon, \forall k \geq 0, \tag{20}$$

here ζ is positive. A CG-method is said to possess this characteristic if there are two constants $\lambda > 0$ and b > 1 that guaranty, for all k,

$$|\beta_k| \geq b \tag{21}$$

if

$$||p_k|| \leq \lambda \text{ ,} then \ |\beta_k| \leq \frac{1}{2b} \ \forall \lambda > 0. \tag{22}$$

3.4 Corollary (Boundedness of θ_k)

Since Assumptions (H) are satisfied, and by using line search with strong Wolfe conditions as described in Eq. (5) the search directions (p_k) are computed through Eqs. From both (14) and (15), we restrict θ_k.

Proof. Utilising the Cauchy-Schwarz inequality and the Lipschitz condition, we obtain

$$|\theta_k| = \left|\frac{p_k^T y_k}{g_k^T g_k}\right| = \frac{|p_k^T y_k|}{|g_k^T g_k|} \leq \frac{|d_k||y_k|}{||g_k||^2} < \frac{\lambda B}{\Upsilon^2} = \overline{b}.$$

3.5 Lemma (Boundedness of α_k)

Assuming that $\forall Y$ on the line segment from y to x, there exists a descent direction p_k and Lipshitz continuity is satisfied, let L be constant for all $\|g_k\|$ [7], thus line search direction satisfies Strong Wolfe condition.

$$\alpha_k \leq \frac{(1-\sigma)|p_k^T g_k|}{L{p_k}^2}. \tag{23}$$

Proof. employing the curvature inequality in Equation (5)

$$\sigma p_k^T g_k \leq p_k^T g_{k+1} \leq -\sigma p_k^T g_k \Rightarrow \sigma p_k^T g_k \leq p_k^T g_{k+1)}. \tag{24}$$

By subtracting $p_k^T g_k$ from both sides of (25) and applying the Lipschitz condition, the following results:

$$(1-\sigma) p_k^T g_k \leq p_k^T (g_{k+1} - g_k) \leq L\alpha_k ||p_k||^2 \tag{25}$$

Given that p_k represents the descending direction and $\sigma \leq 1$, the equation (24) is satisfied:

$$\alpha_k \geq \frac{(1-\sigma)|d_k^T g_k|}{L||d_k||^2}.$$

This lemma is referred to as the Zoutendijk condition [22] and then provide a global convergence proof for any nonlinear conjugate gradient method. From here, which first appeared in the strong Wolfe line search (Eq. (5). We will formulate this condition exactly next in the lemma.

3.6 Lemma

Suppose that Hypotheses (H) hold. Now, we will start analysing the iteration specified by Eqs. (2) and (3), where for each $k \geq 1$, we have descent condition ($p_k^T g_k = p_k^T g_k \leq 0$) and α_k satisfies (5). Subsequently,

$$\sum_{k \geq 0} \frac{(p_k^T g_k)^2}{(||p_k||^2)} < +\infty. \tag{26}$$

Proof. Using the inequality from before in Eq. (5), we obtain

$$f(x_{k+1}) - f(x_k) \leq \delta \alpha_k g_k^T p_k$$

The integration of this with the findings in the Lemma (Boundedness of α_k) produces

$$f_{k+1} - f_k \leq \left[\frac{\delta(1-\sigma)}{L}\right] \frac{(g_k^T p_k)^2}{||p_k||^2}. \tag{27}$$

By utilizing the boundedness of function f as stated in Assumptions (H), we get

$$\sum_{k > 0} \frac{(g_k^T p_k)^2}{||p_k||^2} < \infty. \tag{28}$$

3.7 Theorem.

We assume that Assumption (H) holds and apply Eqs. (2),(3),(14), and (15) where α_k *is using the strong Wolfe line search in Eq. (5),*

$$\liminf_{k\to\infty} ||g_k|| = 0.$$

Proof. The contradiction method is employed to demonstrate that the conclusion is incorrect. Therefore, we assume that $||g_k|| \neq 0$, as previously stated. It is also established that there are constants ζ and Υ both greater than zero. $0 < \zeta \leq ||g_k|| \leq \Upsilon$, for all $k \geq 0$. Now, by calculating the square norm on both sides of our new direction

$$p_{k+1} = -\theta_k g_{k+1} + \beta_k^{MAR} p_k$$

$$\begin{aligned} p_{k+1} &= -\theta_k g_{k+1} + \beta_k^{MAR} p_k \\ &\leq \theta_{k+1}^{M} ||g_{k+1}|| + \beta_{k+1}^{M} ||d_k|| \\ &\leq ||g_{k+1}|| + \beta_{k+1}^{M} ||d_k|| \qquad (By\, the\, Cauchy - Schwarz\, property) \\ &< b\overline{\Upsilon} + b\lambda = C,\ where\, C = b\overline{\Upsilon} + b\lambda. \end{aligned}$$

Since $||p_{k+1}||^2 < (C)^2$, dividing by the quality $||g_{k+1}||^4$, we get

$$\frac{||p_{k+1}||^2}{||g_(k+1)||^4} < \frac{C^2}{||g_{k+1}||^4}.$$

$$\sum_{k=1}^{\infty} \frac{||p_{k+1}||^2}{||g_{k+1}||^4} > C^2 \Upsilon^{-2} = \infty.$$

This is in contradiction with Lemma, then $\liminf_{k\to\infty} ||g_k|| = 0$

4 Numerical Experiment Results

To determine the reliability of the proposed approaches, they are utilized for testing purposes. We compared our newly derived ways with standard approaches BA2 [23] and Malik CGM [20] and use comparable evaluation problems illustrated in Figures 1, 2, and 3. A comparison is made between several widely recognized test functions from CUTE [6], ranging in size from 100 to 1000, with an increasing number 300. The program was developed on Fortran 77 with employing double-precision arithmetic. The algorithm's relative performance is determined by the cumulative number of function evaluations, which usually involve the most expensive component in each iteration, as well as the total number of iterations. The prerequisites for convergence were

$$||g_{k+1}|| \ \leq 1 \times 10^{-5}. \tag{29}$$

A figure is shown to display the proportion P of issues that are completed in less than the desired time for each technique. The graph also shows the proportion of test questions that are solved quickly using a certain approach on the left side, and the percentage of test questions that each method solves correctly on the right side. The curve that demonstrates the greatest effectiveness in terms of problem-solving efficiency is represented as the uppermost curve. Figures 1, 2, and 3 compare MAR-New, BA2, and Malik CG-methods for a total of n various dimensions [100, 400, 700, 1000] for every assessment based on the measure of prefer ability in numerical optimization and the number of iterations and function evaluations; the fourth figure is CPU.

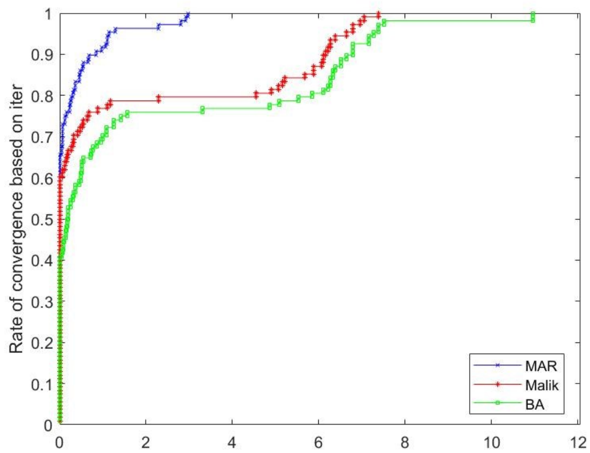

Figure 1: The performance of the compared methods in terms of iter.

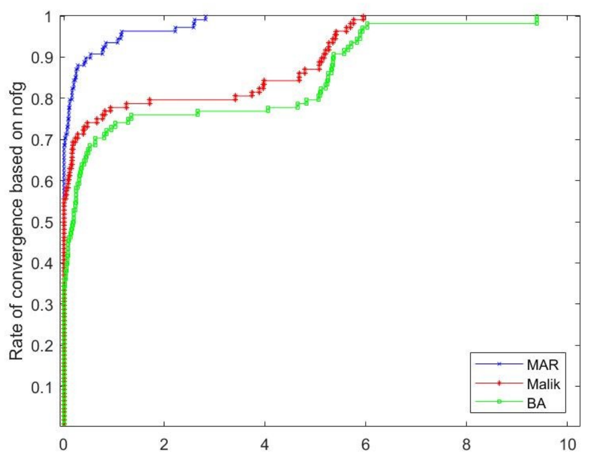

Figure 2: The performance of the compared methods in terms of nofg.

5 Conclusion

Ultimately, we propose robust conjugate gradient techniques (CG) that combine hybrid and spectral components, guided by the parameters β_k^{MAR} and θ_k^{MAR} to determine the search direction. These methods exhibit a notable advantage in ensuring satisfactory descent. Especially in the area of nonlinear dynamics, the gradient-based optimization frequently faces obstacles such as non-convexity, chaotic behavior, or stiff structures. Through a meticulous examination of descent qualities and global convergence for both uniformly convex and general nonlinear functions, we establish that our methodology is

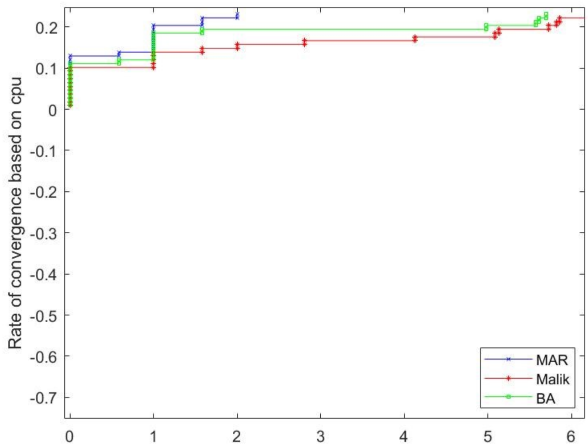

Figure 3: The time performance comparison of the approaches.

appropriately suited for dynamical systems governed by nonlinear equations, a fundamental issue in nonlinear dynamics. Additionally, the algorithms are proven to be globally convergent for both uniformly convex and general non-linear functions. The performance of the proposed CG algorithms against the traditional BA and Malik method is elucidated through some numerical experimentation results based on the essential parameters β_k^{MAR} and θ_k^{MAR}.

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