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Exploring Enhanced Conjugate Gradient Methods: A Novel Family of Techniques for Efficient Unconstrained Minimization

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Abstract

Given that the conjugate gradient method (CGM) is computationally efficient and user-friendly, it is often used to address large-scale, unconstrained minimization issues. Numerous researchers have created new conjugate gradient (CG) update parameters by modifying the initial set, also referred to as classical CGMs. This has resulted in the development of several hybrid approaches. This work's major goal is to create a new family of techniques that can be used to create even more new methods. Consequently, Hestenes-Stiefel's update parameter and a new family involving Polak-Ribiere-Polyak and Liu-Storey CGMs are considered. By changing the parameters of this CGM family, a novel approach that possesses sufficient descent characteristics is obtained. A numerical experiment including many unconstrained minimization problems (UMP) is carried out to assess the novel method's efficacy compared to existing approaches. The result reveals that the new CG approach performs better than the current ones.

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1 Introduction

The goal of an optimization problem is to maximize or minimize a real-valued function by carefully selecting input values from a permitted set and figuring out the function's value. The amount of computational time and computer memory required to solve an optimization issue can be used to quantify the effort involved. The CGM is a widely used iterative strategy for solving optimization problems, particularly those involving large scale data, because of its high numerical efficiency. It was first introduced by Hestenes and Stielel [1] as a technique for handling linear systems of equations.

The early CGMs are referred to as classical CGMs. They are created by the traditional method and serve as the foundation for other CGMs that are built in literature [2, 3]. To reduce the quadratic function, the traditional conjugate gradient algorithm (CGA) was developed based on the following:

$$f(z) = \frac{1}{2} z^T A z - b^T z. \tag{1}$$

It was thought to be computationally costly to apply the CGM for quadratic function minimization to non-quadratic situations because it necessitated the computation of the Hessian matrix at each iteration. Because of variations in their update parameters, numerous CGMs have emerged since Fletcher and Reeves [4] published the first nonlinear CGA. Authors in [1, 4–9] have created some of the earliest sets of classical CG update parameters:

$$\beta_v^{HS} = \frac{g_v^T y_{v-1}}{d_{v-1}^T y_{v-1}}, \tag{2}$$

$$\beta_v^{FR} = \frac{\|g_v\|^2}{\|g_{v-1}\|^2}, \tag{3}$$

$$\beta_v^{PRP} = \frac{g_v^T y_{v-1}}{\|g_{v-1}\|^2}, \tag{4}$$

$$\beta_v^{CD} = \frac{\|g_v\|^2}{-d_{v-1}^T g_{v-1}}, \tag{5}$$

$$\beta_v^{LS} = \frac{g_v^T y_{v-1}}{-d_{v-1}^T g_{v-1}}, \tag{6}$$

and

$$\beta_v^{DY} = \frac{\|g_v\|^2}{d_{v-1}^T y_{v-1}}. \tag{7}$$

The Hestenes-Stiefel, Fletcher-Reeves, Polak-Ribiere-Polyak, conjugate descent, Liu-Storey, and Dai-Yuan techniques are represented by the letters HS, FR, PRP, CD, LS, and DY in the above.

The UMP is typically resolved by a nonlinear CGM:

$$\min f(x), x \in \mathbb{R}^n, \tag{8}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is given as a non-linear and continuously differentiable function and $g = \nabla f$ is the gradient. Starting from an initial guess x_0, a non-linear CGM produces iteratively, a series of points given by:

$$x_{v+1} = x_v + \vartheta_v d_v, \qquad v \geq 0, \tag{9}$$

where ϑ_v denotes the step-length. The search direction, d_v is gotten by:

$$d_v = \begin{cases} -g_v & \text{if } v = 0, \\ -g_v + \beta_v d_{v-1} & \text{if } v \geq 1, \end{cases} \tag{10}$$

where β_v is the CG parameter, which is a scalar.

Selecting the right step size ϑ_v is essential for any CGM. This is true because the selection of the step size, which greatly influences the rate of convergence of any CGM, determines whether a line search method is successful. A careful selection of the line search strategy is necessary to establish a descent direction [10]. For most line search algorithms, the search direction d_v must be descent, i.e., the direction for which $d_v^T g_v < 0$, to guarantee that the function f may be suitably reduced in this direction.

Generally speaking, the line search techniques used to calculate ϑ_v can be precise or imprecise. According to the precise search method, ϑ_v is defined as:

$$\vartheta_v = argmin\{f(x_v + \vartheta d_v); \vartheta \geq 0\}, \tag{11}$$

where ϑ is the value of $\vartheta \geq 0$ that minimizes f along d_v. By solving the differential equation:

$$f'(x_v + \vartheta d_v) = 0, \tag{12}$$

the precise value of ϑ_v is found. This approach is expensive based on the function and gradient evaluation. The shortcomings of the exact line search led to the development of the inexact search method, which computes ϑ_v numerically by guaranteeing a low-cost, acceptable reduction in the value of the goal function. One of the most popular imprecise search methods is the Strong Wolfe (SW) line search, which is characterized by:

$$f(x_v) - f(x_v + \vartheta_v d_v) \geq -\omega \vartheta_v g_v^T d_v, \tag{13}$$

and

$$|g(x_v + \vartheta_v d_v)^T d_v| \leq \gamma |g_v^T d_v|, \tag{14}$$

where $0 \leq \omega \leq \gamma \leq 1$.

The rest of this article is organized as follows: Section 2 reviews the techniques that are currently in use. Section 3 introduces the new parameterized CGM and its algorithm. The analysis of the updated CGM is provided in Section 4. Tables and graphs containing the numerical data are shown and explained in Section 5 while Section 6 contains the conclusion.

2 Review of Existing Methods

In order to improve performance, avoid jamming, and boost convergence, a hybrid CGM is a particular combination of many CGMs [11, 12]. A hybrid CGA was created to utilize and include the enticing features of the traditional CGMs. Hybrid approaches are critical for solving unconstrained optimization problems on a large scale because of their involvement in achieving enhanced computation performance and preserving the strong global convergence properties of the various methods

[13]. This idea makes it possible to switch up the implementation process by using different methods. Two categories of hybrid CGM approaches can be distinguished: mixed methods and methods that combine multiple methods by adding parameters [14], resulting in multiple CGM families. As an example, a family of CGMs with one parameter, suggested by Dai and Yuan [15], is provided by:

$$\beta_v = \frac{\|g_v\|^2}{\alpha_v \|g_{v-1}\|^2 + (1-\alpha_v) d_{v-1}^T y_{v-1}}, \tag{15}$$

where $\alpha_v \in (0, 1)$ is the parameter equation. In this one-parameter family of CGMs, $\alpha_v = 1$ is the same with the FR approach and $\alpha_v = 0$ is equivalent to the DY approach. A two-parameter family of CGMs was proposed by Nazareth [16] and given by:

$$\beta_v = \frac{\rho_v \|g_v\|^2 + (1-\rho_v) g_v^T y_{v-1}}{\eta_v \|g_{v-1}\|^2 + (1-\eta_v) d_{v-1}^T y_{v-1}}, \tag{16}$$

where $\rho_v, \eta_v \in [0, 1]$. The PRP, FR, HS, and DY update parameters are included in this two-parameter family. The six conventional CGMs were incorporated into the three-parameter family by Dai-Yuan in [17], building on the work of Nazareth [16] by adding one more parameter. The following defines the updated parameter that results:

$$\beta_v = \frac{\lambda_v \|g_v\|^2 + (1-\lambda_v) g_v^T y_{v-1}}{(1-\sigma_v-\xi_v) \|g_{v-1}\|^2 + \sigma_v d_{v-1}^T y_{v-1} - \xi_v d_v^T g_v}, \tag{17}$$

where $\sigma_v, \lambda_v \in [0, 1]$ and $\xi_v \in [0, 1-\sigma_v]$.

Djordevic [11, 18] suggested new CG update parameters using a convex combination of both LS and CD techniques as well as HS and FR techniques, yielding the following form:

$$\beta_v^{hyb} = (1-\varsigma_v)\beta_v^{LS} + \varsigma_v \beta_v^{CD},$$

and

$$\beta_v^{hyb} = (1-\varsigma_v)\beta_v^{HS} + \varsigma_v \beta_v^{FR},$$

where ς_v is the hybrid parameter.

According to [13, 19–26], hybrid CGMs have recently been suggested. The novel hybrid CGM, built by convex combination, satisfies the necessary descent condition, according to the author in [19]. This is the formula that yields the new update parameter:

$$\beta_v^{hyb} = (1-\zeta_v)\beta_v^{LS} + \zeta_v \beta_v^{FR}.$$

In [13], The author developed a generic approach using linear combination, which led to the creation of a novel hybrid method in the form of:

$$\beta_v^{NM} = \frac{g_v^T s_{v-1}}{g_{v-1}^T y_{v-1}}. \tag{18}$$

The authors in [23] introduced a new parameter ψ_v by a convex combination of RMIL and MMWU [27, 28] update parameters. The new β_v definition is provided by:

$$\beta_v^{HA} = (1-\psi_v)\,\beta_v^{RMIL} + \psi_v \beta_v^{MMWU}, \tag{19}$$

where

$$\beta_v^{RMIL} = \frac{g_{v+1}^T y_v}{\|d_v\|^2},$$

$$\beta_v^{MMWU} = \frac{\|g_{v+1}\|^2}{\|d_v\|^2},$$

and

$$\psi_v = \frac{\left(s_v^T g_{v+1} - y_v^T g_{v+1}\right)\|d_v\|^2 + \left(g_{v+1}^T y_v\right)\left(y_v^T d_v\right)}{\left(g_{v+1}^T y_v\right)\left(y_v^T d_v\right)}.$$

Much recent research in the development of hybrid CGMs and their characterization have been given in [29–31].

In this study, a novel parameterized CGM is proposed by utilizing a linear combination of some of the current CGMs. This work is unique in that it does not impose restrictions on the values of the parameters, which permits both the recovery of the current methods and the creation of new ones.

3 The New CGM

This section initially proposes a novel family of CGMs that may be among the first sets of CGMs with comparable numerators. The developers of these current traditional techniques are [1,5,6,8]. The update parameter that results is provided by:

$$\beta_v^{NF``(1)} = \frac{\nu g_v^T y_{v-1}}{\lambda_1 d_{v-1}^T y_{v-1} + \lambda_2 \|g_{v-1}\|^2 + \lambda_3 d_{v-1}^T g_{v-1}}. \tag{20}$$

Using $y_{v-1} = g_v - g_{v-1}$ in the numerator of (20), a more general update parameter of the form:

$$\beta_v^{NF(2)} = \frac{\nu_1 \|g_v\|^2 + \nu_2 g_v^T g_{v-1}}{\zeta_1 d_{v-1}^T y_{v-1} + \zeta_2 \|g_{v-1}\|^2 + \zeta_3 d_{v-1}^T g_{v-1}}, \tag{21}$$

is presented, where the parameters $\nu_i, \zeta_j, i = 1,2, j = 1,2,3 \in \mathbb{R}$, $d_{v-1}, g_v, g_{v-1}, y_{v-1}$, are vectors and T represents transpose.

Definition 3.1. *[32] Given a vector space V containing elements $r_1, \cdots, r_n$ and scalars $\kappa_1, \cdots, \kappa_n$ over a field K, then the span of a set S of vectors in V can be defined as the set of all finite linear combination of elements of S, i.e.,*

$$Span(S) = \left\{ \sum_{i=1}^{k} \kappa_i r_i | K \in \mathbb{N}, r_i \in S, \kappa_i \in K \right\}.$$

Therefore $V = Span\{r_1, r_2, \cdots, r_n\}$, and V is said to be spanned by $r_1, r_2, \cdots, r_n$.

3.1 Formula for existing and new CGMs

Let A and B be the set of the numerator and denominator terms of (21) i.e.,

$$A = \{a_1, a_2, \cdots, a_n\},$$

$$B = \{b_1, b_2, \cdots, b_n\},$$

where the numerator and denominator terms $a_i, i = 1, \cdots, n$ and $b_i, i = 1, \cdots, n$ are respectively $\|g_v\|^2, g_v^T g_{v-1}, d_{v-1}^T y_{v-1}, \|g_{v-1}\|^2$, and $d_{v-1}^T g_{v-1}$. By Definition 3.1,

$$Span(A) = \left\{ \sum_{i=1}^{n} \nu_i a_i, \qquad \nu_i \in \mathbb{R}, \qquad a_i \in A \right\},$$

and

$$Span(B) = \left\{ \sum_{i=1}^{n} \zeta_i b_i, \qquad \zeta_i \in \mathbb{R}, \qquad b_i \in B \right\}.$$

Let the set of both existing and new methods be denoted by M, then:

$$M = \left\{ \frac{p}{q} | p \in Span(A), \quad q \in Span(B) \right\}. \tag{22}$$

By using the formula (22), the existing methods i.e. the HS, PRP and LS methods can be recovered and new methods can also be generated from (21) as follows:

By letting $\nu_1 = 1$, $\nu_2 = -1$, $\zeta_1 = 1$, others zero, method HS is recovered.
By making $\nu_1 = 1$, $\nu_2 = -1$, $\zeta_2 = 1$, others zero, method PRP is recovered.
By making $\nu_1 = 1$, $\nu_2 = -1$, $\zeta_3 = -1$, others zero, method LS is recovered.

Therefore for ease of analysis and implementation, a new method is generated from (21) by letting $\nu_2 = 1$, $\zeta_2 = 1$, others zero, resulting in the following method:

$$\beta_v^{NGM} = \frac{g_v^T g_{v-1}}{\|g_{v-1}\|^2}, \tag{23}$$

where NGM refers to new gradient method. The following algorithm describes the newly generated CGM.

NGM Algorithm

Step 1: Given that $x_v \in \mathbb{R}^n, v = 0, \epsilon \geq 0$, set $d_v = -g_v$, stop if $\|g_v\| \leq \epsilon$.
Step 2: Determine the stepsize ϑ_v by SW inexact line search given by (13) and

(14).
Step 3: Let x_v be determined by (9), $g_v = g(x_v)$, stop if $\|g_v\| \leq \epsilon$.
Step 4: Calculate β_v by (23) and produce d_v by (10).
Step 5: Make $v := v + 1$, and go back to step 2.

4 Analysis of the NGM Method

The following lemmas will be useful in carrying out the sufficient descent analysis of β_v^{NGM}.

Lemma 4.1. *For the Conjugate Gradient Method, the following holds:*

$$g_v^T d_{v-1} = 0. \tag{24}$$

Proof. This can be found in Chong and Zak [33]. □

Lemma 4.2. *The NGM update parameter satisfies the sufficient descent criterion, i.e.,*

$$g_v^T d_v \leq -\varpi \|g_v\|^2, \qquad 0 < \varpi \leq 1. \tag{25}$$

Proof. By (10) and (23),

$$\begin{aligned} g_v^T d_v &= -g_v^T g_v + \beta_v^{NGM} \left(g_v^T d_{v-1}\right), \\ &= -\|g_v\|^2 + \frac{g_v^T g_{v-1}}{\|g_{v-1}\|^2} \left(g_v^T d_{v-1}\right). \end{aligned}$$

Expressing the second term on the right hand side (RHS) in the form of Cauchy-Schwartz inequality $k^T l \leq \frac{1}{2}(\|k\|^2 + \|l\|^2)$ by letting $k = \frac{1}{\sqrt{3}} g_v$, and $l = \frac{\sqrt{3} g_{v-1}\left(g_v^T d_{v-1}\right)}{\|g_{v-1}\|^2}$, we have:

$$\begin{aligned}\frac{g_v^T g_{v-1}}{\|g_{v-1}\|^2}\left(g_v^T d_{v-1}\right) &\leq \frac{1}{2}\left[\left\|\frac{1}{\sqrt{3}}g_v\right\|^2 + \left\|\frac{\sqrt{3}g_{v-1}\left(g_v^T d_{v-1}\right)}{\|g_{v-1}\|^2}\right\|^2\right], \\ &\leq \frac{1}{2}\left[\frac{1}{3}\|g_v\|^2 + \frac{3(g_v^T d_{v-1})^2}{\|g_{v-1}\|^4}\right].\end{aligned}$$

By Lemma (4.1), the second term in the above vanishes and therefore,

$$\frac{g_v^T g_{v-1}}{\|g_{v-1}\|^2}\left(g_v^T d_{v-1}\right) \leq \frac{1}{6}\|g_v\|^2,$$

and

$$\begin{aligned}g_v^T d_v &= -\|g_v\|^2 + \frac{g_v^T g_{v-1}}{\|g_{v-1}\|^2}\left(g_v^T d_{v-1}\right), \\ &\leq -\|g_v\|^2 + \frac{1}{6}\|g_v\|^2, \\ &\leq -\frac{5}{6}\|g_v\|^2.\end{aligned}$$

□

Thus, the NGM method satisfies (25) with $\varpi = \frac{5}{6}$.

5 Numerical Results and Discussion

The NGM algorithm's results on a series of test problems are presented in this section. Using the same test problems that were chosen from Bongartz et al. [34] and Andrei [35], this algorithm's reliability was evaluated in comparison to the NM method [13] and the HA method [23].

In total, 80 computations were performed by solving twenty (20) unconstrained test functions with dimensions ranging from 500 to 10,000. The computation was performed using the SW line search, and the CGA codes were written using MATLAB software on a computer running Windows 10 Pro with a 2.16 GHz processor, 4 GB of RAM, and a CGA code generator. A failure (F) was identified if the condition $\|g_v\| \leq 10^{-6}$ was not satisfied after 2000 iterations.

Table 2 shows in detail the numerical results for the test functions (TF) specified in Table 1, which include the dimensions of the solved problems (DIM), iteration counts (ITER), and the computer processing time (CPUT). The solved test functions and their sources are shown in Table 1. Figures 1 and 2, correspondingly, display the performance outcomes. Dolan and More's performance profile was used to evaluate these [36]. The NGM approach performs better than the NM and HA methods, as evidenced by the fact that it was able to solve 84% of the test problems successfully. On the other hand, only roughly 35% of the test problems could be resolved with the HA approach, while 56% could be resolved with the NM approach.

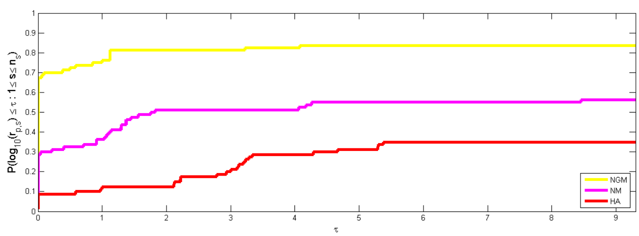

Figure 1: Comparing the NGM, NM and HA methods with respect to number of iterations.

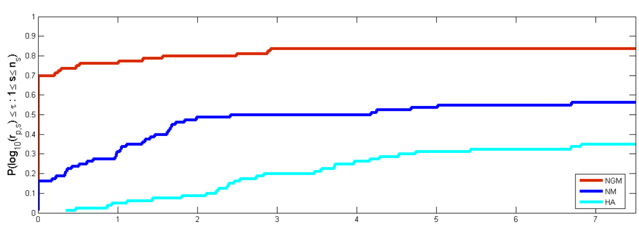

Figure 2: Comparing the NGM, NM and HA methods in terms of Computational time.

Table 1: Solved test functions together with their origins

S/N	TF	Origins
1	"Extended Block Diagonal BD1	Andrei (2008)
2	Power	Andrei (2008)
3	Arwhead	Bongartz *et al.* (1995)
4	Diagonal 5	Andrei (2008)
5	Qf1	Andrei (2008)
6	Qf2	Andrei (2008)
7	Chebyquad	Andrei (2008)
8	Diagonal 4	Andrei (2008)
9	Staircase1	Andrei (2008)
10	Staircase2	Andrei (2008)
11	Extended Beale	Andrei (2008)
12	Extended Freudenstein and Roth	Andrei (2008)
13	MODF COSINE	Bongartz *et al.* (1995)
14	MODF SINE	Bongartz *et al.* (1995)
15	MDF EXPLIN 1	Bongartz *et al.* (1995)
16	RMODF COSINE	Bongartz *et al.* (1995)
17	RMDF GENHUMPS	Bongartz *et al.* (1995)
18	Ext MCCORMCK	Bongartz *et al.* (1995)
19	Extended Three Exponential Terms	Andrei (2008)
20	Extended Quadratic Penalty QP2	Andrei (2008)"

Table 2: ITER and CPUT outputs for NGM, HA and NM methods

		CPUT			**ITER**		
TF	**DIM**	**“NGM**	**NM**	**HA**	**NGM**	**NM**	**HA**
1	500	0.741	0.098	F	37	17	F
	1000	0.743	0.101	F	37	17	F
	5000	0.78	0.264	F	37	17	F
	10000	1.035	0.417	F	37	17	F
2	500	1.189	0.211	0.91	27	26	51
	1000	F	F	F	F	F	F
	5000	F	F	F	F	F	F
	10000	F	F	F	F	F	F
3	500	10.152	8.31	F	493	1751	F
	1000	11.627	F	F	550	F	F
	5000	F	F	F	F	F	F
	10000	F	F	F	F	F	F
4	500	0.306	0.213	F	8	15	F
	1000	0.159	0.114	F	8	15	F
	5000	0.229	0.726	F	8	27	F
	10000	0.253	6.489	F	8	133	F
5	500	30.029	F	F	658	F	F
	1000	47.192	F	F	1307	F	F
	5000	43.164	F	F	1495	F	F
	10000	F	F	F	F	F	F
6	500	F	F	F	F	F	F
	1000	F	F	F	F	F	F
	5000	F	F	F	F	F	F
	10000	F	F	F	F	F	F
7	500	0.063	0.208	0.984	24	17	431
	1000	0.078	0.31	1.794	36	20	829
	5000	0.271	0.234	F	84	9	F
	10000	0.565	0.28	F	118	7	F
8	500	0.102	0.211	1.13	20	41	93
	1000	0.124	0.267	F	20	42	F
	5000	0.347	0.921	9.244	20	44	160
	10000	0.67	1.329	F	21	45	F

Table 2 cont'd

		CPUT			ITER		
TF	**DIM**	**NGM**	**NM**	**HA**	**NGM**	**NM**	**HA**
9	500	0.017	0.042	0.046	1	1	1
	1000	0.019	0.029	0.036	1	1	1
	5000	0.022	0.043	0.028	1	1	1
	10000	0.024	0.028	0.052	1	1	1
10	500	0.158	2.854	16.257	33	634	1301
	1000	0.193	3.661	21.75	34	613	1326
	5000	0.371	0.312	2.087	30	23	46
	10000	F	F	F	F	F	F
11	500	4.6	9.398	F	420	1034	F
	1000	6.214	19.33	F	429	1052	F
	5000	27.751	76.547	153.255	403	1118	379
	10000	58.233	147.846	F	442	1145	F
12	500	5.912	F	F	723	F	F
	1000	13.94	F	F	961	F	F
	5000	49.332	F	F	961	F	F
	10000	78.846	F	F	916	F	F
13	500	0.107	F	0.374	19	F	131
	1000	0.065	F	0.377	18	F	137
	5000	0.142	F	1.011	18	F	154
	10000	0.449	F	2.326	36	F	168
14	500	0.047	4.86	0.221	5	1757	47
	1000	0.02	0.064	0.235	3	2	39
	5000	0.023	0.029	0.042	1	1	1
	10000	0.031	0.035	0.043	1	1	1
15	500	0.041	0.081	0.538	11	11	96
	1000	0.041	0.126	0.542	11	11	101
	5000	0.11	0.585	2.142	11	18	107
	10000	0.099	3.191	4.251	11	30	111
16	500	0.089	0.113	F	22	29	F
	1000	0.069	0.247	F	22	57	F
	5000	0.2	F	F	25	F	F
	10000	0.283	F	F	25	F	F
17	500	0.126	0.18	F	32	16	F
	1000	F	0.259	1.359	F	17	74
	5000	F	1.284	F	F	18	F
	10000	0.714	F	F	21	F	F
18	500	0.097	0.13	0.466	28	28	42
	1000	0.095	0.153	1.699	25	29	108
	5000	0.544	F	F	44	F	F
	10000	2.848	F	F	96	F	F
19	500	0.187	0.241	F	40	41	F
	1000	0.345	F	F	53	F	F
	5000	9.848	F	F	271	F	F
	10000	42.96	F	F	510	F	F
20	500	2.739	F	F	467	F	F
	1000	8.995	F	F	604	F	F
	5000	20.052	F	F	444	F	F
	10000	66.502	F	F	724	F	F"

6 Conclusion

This paper presents a new family of parameterized CGMs that was created by linearly combining three traditional CGMs that already existed and had similar numerators. By changing the values of the parameters in the new family, this strategy has the potential to generate an infinite number of new methods. Consequently, it was demonstrated that a newly selected CGM had the appropriate descent property. Numerical comparisons between the new method and three current CGMs demonstrate that the new method performs better in terms of computation time and iteration numbers. This is indicated by the potential for the new family to produce a CGM that performs better than any of the current CGMs. Thus, more research into the new enhanced family of CG Methods is required. Future studies will concentrate on the new method's global convergence.

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