

# A new conjugate gradient for unconstrained optimization problems and its applications in neural networks

Alaa Luqman Ibrahim<sup>1</sup>, Mohammed Guhdar Mohammed<sup>2</sup>

<sup>1</sup>Department of Mathematics, Faculty of Science, University of Zakho, Zakho, Iraq

<sup>2</sup>Department of Computer Science, Faculty of Science, University of Zakho, Zakho, Iraq

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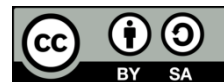
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## ABSTRACT

We introduce a novel efficient and effective conjugate gradient approach for large-scale unconstrained optimization problems. The primary goal is to improve the conjugate gradient method's search direction in order to propose a new, more active method based on the modified vector  $v_k^*$ , which is dependent on the step size of Barzilai and Borwein. The suggested algorithm features the following traits: (i) The ability to achieve global convergence; (ii) numerical results for large-scale functions show that the proposed algorithm is superior to other comparable optimization methods according to the number of iterations (NI) and the number of functions evaluated (NF); and (iii) training neural networks is done to improve their performance.

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## Corresponding Author:

Alaa Luqman Ibrahim

Department of Mathematics, Faculty of Science, University of Zakho

Zakho, Kurdistan Region, Iraq

Email: alaa.ibrahim@uoz.edu.krd

## 1. INTRODUCTION

In this section, we will offer a concise yet comprehensive overview of unconstrained optimization and its intersection with neural networks. Unconstrained optimization refers to the mathematical techniques and algorithms used to find the optimal solution of a problem without any constraints on the decision variables. It plays a pivotal role in various machine learning and deep learning applications, especially when training neural networks. Neural networks, on the other hand, are a class of machine learning models inspired by the human brain, consisting of interconnected nodes and layers that learn patterns from data.

– Unconstrained optimization

Take into account the following unconstrained optimization problem;

$$\text{Min}\{f(x): x \in R^n\} \quad (1)$$

where a function  $f: R^n \rightarrow R$  be continuously differentiable  $R^n$  denotes an n-dimensional euclidean space. Numerous real-world application areas exist for the aforementioned issue, including economics, biology, and engineering. The nonlinear conjugate gradient (CG) method is one of the most well-known and successful methods for (1). Starting with an initial guess of  $x_0 \in R^n$ , we should create a sequence of  $\{x_k\}$  such;

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

where  $\alpha_k > 0$  is achieved by line search and the direction  $d_k$  are generated as;

$$d_{k+1} = \begin{cases} -g_{k+1}, & k = 0 \\ -g_{k+1} + \beta_k d_k, & k > 0 \end{cases} \quad (3)$$

where  $g_k = \nabla f(x_k)$  and  $\beta_k$  is a scalar parameter [1], [2]. In addition, for many years, researchers focused researchers to proposed variety expression of  $\beta_k$  as well as  $d_{k+1}$  (see, e.g., [2]–[10]) to increasing more efficient and successful conjugate gradient algorithms. Perry [11] suggested a parameter of conjugate gradient defined as;

$$\beta_k^{Perry} = \frac{g_{k+1}^T (y_k - v_k)}{d_k^T y_k} \quad (4)$$

where  $y_k = g_{k+1} - g_k$  and  $v_k = x_{k+1} - x_k$ . When calculating the step-size, it is argued that  $\alpha_k$  satisfies any of the conditions for a line search [12]–[14]. In this study, we employ a strong wolfe line search.

$$f(x_k + \alpha_k d_k) \leq f(x) + \delta \alpha_k g_k^T d_k, 0 \leq \delta \leq \frac{1}{2} \quad (5)$$

$$|d_k^T g(x_k + \alpha_k d_k)| \leq -\sigma g_k^T d_k, \delta \leq \sigma \leq 1 \quad (6)$$

#### – Summary of artificial neural network history

In order to execute network pattern decision making, ANN is inspired by the biological human brain, which is made up of up to 60 trillion interconnected groups of neurons. Based on this fundamental concept, an artificial neural network's construction starts with a collection of basic, interconnected neurons that function as a single processor. Based on the neuron model developed by McCulloch and Pits, the perceptron notion has been introduced [15]. A single layer of input, process, and output elements forms the basis of an ANN. In order to generate the best outcome for any datasets or issue segments, ANN acts as a complicated mathematical formulation starting from a very fundamental understanding of the information processing cycle. Neurons should be checked using feed-forward and backward algorithms in order to complete a network cycle. Back propagation or backward algorithms are the topics that have received the most attention from researchers in the past and now. The machine learning component of ANN that has gained the most attention in current research and development. Machine learning refers to the capability of a computer to comprehend data structure utilizing mathematical or statistical models. Artificial neural networks, on the other hand, require additional processes in order to deal with complex patterns in vast volumes of data. Deep methodological learning and structured algorithms are needed for this. In its execution process, ANN uses a variety of methodologies, including supervised learning, unsupervised learning, and reinforcement learning. Neural network learning techniques are still being studied and recognized by communities as of this writing. It quickly became well-liked in machine learning [16]–[18] and is frequently considered to be more effective because to its exceptional capacity for self-adaptation and self-learning;  $net_j^l = \sum_{i=1}^{N_{l-1}} w_{ij}^{l-1,l} y_i^{l-1} + b_j^l, y_i^l = f(net_j^l)$  The determines how a FNN works.

Where the sum of its weighted inputs is  $net_j^l$ , for the  $j^{th}$  node in the  $l^{th}$  layer ( $j = 1, \dots, N_l$ ),  $w_{ij}^{l-1,l}$  are the weights from the  $i^{th}$  neuron at the layer to the  $j^{th}$  neuron at the  $l^{th}$  layer,  $b_j^l$  is the bias of the  $j^{th}$  neuron at the  $l^{th}$  layer,  $y_i^l$  is the output of the  $j^{th}$  neuron that belongs to the  $l^{th}$  layer, and  $f(net_j^l)$ , is the  $j^{th}$  neuron activation function.

The core concept of neural network training can be expressed as a nonlinear unconstrained optimization problem. In order to globally reduce the difference between the network's actual output and the planned output for all examples in the training set, a neural network is trained by incrementally changing its weights [19]. The training procedure may therefore be described mathematically as the minimization of the error function  $E(w)$ , which is defined by the sum of square differences between the actual output of the FNN, i.e.,

$$E(w) = \sum_{p=1}^P \sum_{j=1}^{N_l} (y_j^{l-1} - t_{j,p})^2 \quad (7)$$

where  $w \in R^n$  is the vector network weights and the number of patterns used in the training set represented by  $P$ . [3]–[20].

The remainder of the paper is formatted as follows: we present our strategy for acquiring the new propose CG algorithm acquiring in section 2. The descent and sufficient descent property of our approach and the global convergence property were tested in section 3. In section 4, some numerical experiments to new CG algorithm and the HS algorithm are reported. In section 5, presents the application of the CG algorithm for training neural networks; the paper's conclusion and algorithm's characters were listed in section 5.

## 2. NEW CONJUGATE GRADIENT ALGORITHM FOR SMOOTH PROBLEMS

The nonlinear conjugate gradient algorithm is a well-known example of an efficient technique for optimization problems due to its low storage requirements and easy structure. It encourages us to conduct additional research and develop a modified conjugate gradient formula for the unrestricted optimization model. In this section, we will submit a new coefficient conjugate gradient algorithm for unconstrained minimization problems depend on the modified vector which is defined as:  $v_k^* = \frac{1}{\alpha_k^{BB}} v_k - \frac{\theta}{\alpha_k^{BB}} v_k$ , where  $\theta \in (0,1)$  and  $\alpha_k^{BB} = \frac{v_k^T v_k}{y_k^T v_k}$ , see [21].

$$\text{So, we have } v_k^* = (1 - \theta) \frac{y_k^T v_k}{v_k^T v_k} v_k \tag{8}$$

More precisely, the conjugate gradient algorithms are iterative methods of the form given by (1) and (2). The major idea of our new algorithm is to improve the performance of CG algorithm Perry by replacing  $v_k$  by  $v_k^*$  in (4). Then,

$$\beta_k^{New} = \frac{g_{k+1}^T (y_k - v_k^*)}{d_k^T y_k} = \frac{g_{k+1}^T y_k}{d_k^T y_k} - (1 - \theta) \frac{y_k^T v_k}{v_k^T v_k} \frac{g_{k+1}^T v_k}{d_k^T y_k} \tag{9}$$

Algorithm steps: iterative gradient method for unconstrained optimization:

- 1) Given an initial point  $x_0 \in R^n$
- 2) Set  $d_0 = -g_0$ ,  $k = 0$ . If  $\|g_k\| = 0$  then stop, otherwise go to step 3.
- 3) Compute the step size  $\alpha_k$  by using minimize  $f(x_k + \alpha_k d_k)$ .
- 4) Set  $x_{k+1} = x_k + \alpha_k d_k$ .
- 5) Determine  $g_{k+1}$ , if  $\|g_{k+1}\| \leq 10^{-5}$  stop, else go to step 6.
- 6) Compute  $d_{k+1}$  by (2) and  $\beta_k^{New}$  from (9).
- 7) If  $\|g_{k+1}\|^2 \leq \frac{|g_k^T g_{k+1}|}{0.2}$  is satisfied go to step 3, else  $k = k + 1$  and go to step 3.

## 3. CHARACTERISTICS OF ALGORITHMS

The properties of the descent and sufficient descent, as well as global convergence of the new algorithm, are stated in this section:

**Theorem 3.1:** if the search direction  $d_{k+1}$  is generated by (2) and  $\beta_k^{New}$  from (9), then,

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

**Proof:** multiply both sides of (2) by  $g_{k+1}$  where  $\beta_k^{New}$  defined in (9), to obtain,

$$g_{k+1}^T d_{k+1} = -g_{k+1}^T g_{k+1} + \frac{g_{k+1}^T y_k}{d_k^T y_k} g_{k+1}^T d_k - (1 - \theta) \frac{y_k^T v_k}{v_k^T v_k} \frac{g_{k+1}^T v_k}{d_k^T y_k} g_{k+1}^T d_k \tag{10}$$

if the above search direction is exact, then it is satisfying the descent condition i.e.,

$$g_{k+1}^T d_{k+1} = -\|g_{k+1}\|^2 \leq 0$$

however, if the search direction (10) is inexact (i.e.)  $g_{k+1}^T d_k \neq 0$ . We get to the conclusion that the first two terms in (10) satisfy the requirement for descent, i.e.,

$$-g_{k+1}^T g_{k+1} + \frac{g_{k+1}^T y_k}{d_k^T y_k} g_{k+1}^T d_k \leq 0 \tag{11}$$

because  $g_{k+1}^T d_k \leq d_k^T y_k$  and  $g_{k+1}^T y_k = g_{k+1}^T g_{k+1} - g_{k+1}^T g_k$  and  $0.2\|g_{k+1}\|^2 \leq |g_k^T g_{k+1}|$  we have since,  $g_{k+1}^T v_k = \alpha_k g_{k+1}^T d_k$ . Therefore, we can present the (10) as,

$$g_{k+1}^T d_{k+1} \leq -(1 - \theta) \alpha_k \frac{y_k^T v_k}{v_k^T v_k} \frac{g_{k+1}^T d_k}{d_k^T y_k} (g_{k+1}^T d_k)^2 \tag{12}$$

clearly,  $\alpha_k, (1 - \theta), y_k^T v_k, v_k^T v_k, d_k^T y_k$  and  $(g_{k+1}^T d_k)^2$  are non-negative. So, we have  $g_{k+1}^T d_{k+1} \leq 0$ .

**Theorem 3.2:** the direction  $d_{k+1}$  defined by (2) and  $\beta_k^{New}$  from (9); then there exists a positive  $\mu > 0$  satisfying.

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

**Proof:** it is clear from Theorem (3.1) that the first two components of (10) are less than or equal to zero after multiplying the new search direction (2) and (9) by  $g_{k+1}$ , and from (12), we obtain,

$$g_{k+1}^T d_{k+1} \leq -(1-\theta)\alpha_k \frac{y_k^T v_k \|d_k\|^2}{v_k^T v_k d_k^T y_k} \|g_{k+1}\|^2 \quad (13)$$

Let  $\mu = -(1-\theta)\alpha_k \frac{y_k^T v_k \|d_k\|^2}{v_k^T v_k d_k^T y_k}$  which is positive, then,  $g_{k+1}^T d_{k+1} \leq -\mu \|g_{k+1}\|^2$ , the proof is completed. we propose the following mild assumptions to get aiming at achieving global convergence.

**Assumption:** [22], [23]

- I. The level set  $\delta = \{x | f(x) \leq f(x_0)\}$  is bounded.
- II. In some neighborhood  $N$  of  $\delta$ ,  $f$  is continuously differentiable, and its gradient is lipschitz continuous with Lipschitz constant  $\delta > 0$ , i.e.,

$$\|g(x) - g(y)\| \leq \delta \|x - y\| \quad \forall x, y \in \delta$$

from the above assumptions, that there exists a positive constant  $b$  such that.

$$\|g(x)\| \leq b \quad \forall x \in \delta. \quad (14)$$

following is established for the global convergence of the new algorithm based on the discussion above.

**Lemma 3.1:** [24] Let assumptions (I)–(II) hold. Consider the methods (1) and (2), where  $d_{k+1}$  is a descent direction and  $\alpha_k$  satisfies the standard wolfe line search. If,

$$\sum_{k \geq 1} \frac{1}{\|d_{k+1}\|^2} = \infty. \text{ Then, } \liminf_{k \rightarrow \infty} \|g_{k+1}\| = 0$$

based on the above discussion the global convergence of new algorithm is established as follows.

**Theorem 2.3:** if assumptions (I) and (II) are valid and Algorithm 2.1 generates the corresponding sequences of  $\{x_k\}$ ,  $\{d_k\}$ ,  $\{g_k\}$ ,  $\{\alpha_k\}$ , then we get to the conclusion that,

$$\liminf_{k \rightarrow \infty} \|g_{k+1}\| = 0$$

**Proof:** from (2) and (9), we have,

$$\|d_{k+1}\| \leq \|g_{k+1}\| + \left| \frac{g_{k+1}^T y_k}{d_k^T y_k} - (1-\theta) \frac{y_k^T v_k g_{k+1}^T v_k}{v_k^T v_k d_k^T y_k} \right| \|d_k\| \quad (15)$$

$$\|d_{k+1}\| \leq \|g_{k+1}\| + \left( \left| \frac{g_{k+1}^T y_k}{d_k^T y_k} \right| + (1-\theta) \left| \frac{y_k^T v_k g_{k+1}^T v_k}{v_k^T v_k d_k^T y_k} \right| \right) \|d_k\| \quad (16)$$

since  $g_{k+1}^T v_k \leq \alpha_k d_k^T y_k$  and by using (14), also from lipschitz condition  $\|y_k\| \leq L \|v_k\|$  and  $g_{k+1}^T y_k \leq L g_{k+1}^T d_k$  where  $L > 0$ , we have,

$$\|d_{k+1}\| \leq M + (L + (1-\theta)\alpha_k L) \|d_k\| \quad (17)$$

since,  $\|v_k\| = \|x - x_k\|$ ,  $D = \max\{\|x - x_k\|\}, \forall x, x_k \in R\}$ . Hence (17) becomes  $\|d_{k+1}\| \leq M + ((1-\theta)\alpha_k)DL = \beta$

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

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

by using lemma (3.1), we get  $\lim_{k \rightarrow \infty} \inf \|g_k\| = 0$ . Which completes the proof.

**4. NUMERICAL RESULTS FOR UNCONSTRAINED OPTIMIZATION**

This part focuses on evaluating how well our approach for resolving optimization issues works in practice. We contrast HS method with our novel algorithm. Well-known test functions [25] with varying dimensionality were used in the comparison testing. Fortran 95 is used to write all program lines. The cubic interpolation method utilized in the line search routine utilised function and gradient values. The outcomes shown in Table 1 depend on the number of iterations (NI) and functions (NF). Table 2 experimental findings support the claim that the new method outperforms the HS algorithm in terms of number of iterations, and or number of functions.

Table 1. The results for the HS and New CG methods on the tested problems

| Test function | n     | HS  |     | New CG |     | (Continued)  | Test function | n   | HS    |       | New CG |       |
|---------------|-------|-----|-----|--------|-----|--------------|---------------|-----|-------|-------|--------|-------|
|               |       | NI  | NF  | NI     | NF  |              |               |     | NI    | NF    | NI     | NF    |
| G-Cantrel     | 4     | 22  | 159 | 21     | 150 | Miele        | 4             | 28  | 85    | 28    | 85     |       |
|               | 10    | 22  | 159 | 21     | 150 |              | 10            | 31  | 102   | 28    | 85     |       |
|               | 100   | 22  | 159 | 22     | 163 |              | 100           | 33  | 114   | 31    | 102    |       |
|               | 500   | 23  | 171 | 22     | 163 |              | 500           | 40  | 146   | 39    | 139    |       |
|               | 1,000 | 23  | 171 | 22     | 163 |              | 1,000         | 46  | 176   | 39    | 139    |       |
|               | 5,000 | 28  | 248 | 23     | 176 |              | 5,000         | 54  | 211   | 39    | 139    |       |
| G-Wolfe       | 4     | 11  | 24  | 11     | 24  | G-Wood       | 4             | 30  | 68    | 26    | 61     |       |
|               | 10    | 32  | 65  | 32     | 65  |              | 10            | 30  | 68    | 26    | 61     |       |
|               | 100   | 49  | 99  | 49     | 99  |              | 100           | 30  | 68    | 26    | 61     |       |
|               | 500   | 52  | 105 | 52     | 105 |              | 500           | 30  | 68    | 26    | 61     |       |
|               | 1,000 | 70  | 141 | 60     | 121 |              | 1,000         | 30  | 68    | 28    | 65     |       |
|               | 5,000 | 165 | 348 | 165    | 345 |              | 5,000         | 30  | 68    | 28    | 65     |       |
| Powell        | 4     | 37  | 102 | 33     | 91  | Non-Diagonal | 4             | 24  | 64    | 24    | 64     |       |
|               | 10    | 37  | 102 | 33     | 91  |              | 10            | 26  | 72    | 26    | 72     |       |
|               | 100   | 40  | 117 | 36     | 106 |              | 100           | 29  | 79    | 29    | 79     |       |
|               | 500   | 44  | 136 | 36     | 106 |              | 500           | F   | F     | 29    | 82     |       |
|               | 1,000 | 44  | 136 | 36     | 106 |              | 1,000         | 29  | 79    | 29    | 79     |       |
|               | 5,000 | 44  | 136 | 36     | 106 |              | 5,000         | 30  | 81    | 30    | 81     |       |
| Rosen         | 4     | 30  | 83  | 30     | 83  | OSP          | 4             | 8   | 45    | 8     | 44     |       |
|               | 10    | 30  | 83  | 30     | 83  |              | 10            | 13  | 58    | 13    | 60     |       |
|               | 100   | 30  | 83  | 30     | 83  |              | 100           | 49  | 185   | 49    | 173    |       |
|               | 500   | 30  | 83  | 30     | 83  |              | 500           | 112 | 353   | 107   | 341    |       |
|               | 1,000 | 30  | 83  | 30     | 83  |              | 1,000         | 156 | 475   | 150   | 450    |       |
|               | 5,000 | 30  | 83  | 30     | 83  |              | 5,000         | 256 | 774   | 256   | 765    |       |
| Total         |       |     |     |        |     |              |               |     | 2,147 | 6,747 | 2,004  | 6,181 |

Notes:

- I. The letter F in the previous table denotes that a technique to determine the minimum was unsuccessful.
- II. We assumed that the HS failure result was worth twice as much as the new CG findings.

Table 2. The percentage of improvement between the HS and New CG methods

| Tools | HS   | New CG   |
|-------|------|----------|
| NI    | 100% | 93.3395% |
| NF    | 100% | 91.6111% |

Algorithm 2.1 applications for training neural networks

This section presents the experimental numerical findings used to analyze and compare the effectiveness of the traditional and novel CG methods for training neural networks. We specifically look into how the HS method performed in comparison to the new CG method throughout the course of the program’s five times implementation. The conjugate gradient MATLAB neural network toolbox version 8.1 and MATLAB (2013a) are used to implement the methods. To reduce the value of the error’s function, the network is trained until the mean squares of the errors are below the error goal. We evaluate all methods using the identical initial weights, which were generated at random from the range (0, 1) where the problems:

- Input P = [-1, -1, 2, 2, 0, 5, 0, 5] and the target T = [-1, -1, 1, 1], the target error has been set to  $1 \times 10^{-20}$  and the maximum epochs to 1,000 as used.

- Input continuous trigonometric function  $f(x) = \sin(x) + \cos(2x)$  where  $x \in [0, \pi]$  and the target error has been set to  $1 \times 10^{-20}$  and the maximum epochs to 1,000 as used.

The results of the training methods are present in the Table 3 and Figures 1 to 4.

Table 3. Performance evaluation of new and conventional methods for training neural networks

| Methods   | No. Running | Epochs | CPU time (s)/Epoch | Gradient |
|-----------|-------------|--------|--------------------|----------|
| Problem 1 |             |        |                    |          |
| Standard  | 1           | 1,000  | 0:00:04            | 0.000376 |
|           | 2           | 34     | 0:00:00            | 0.000239 |
|           | 3           | 41     | 0:00:00            | 0.000173 |
|           | 4           | 21     | 0:00:00            | 0.000209 |
|           | 5           | 38     | 0:00:00            | 0.000157 |
| New CG    | 1           | 8      | 0:00:01            | 0.0581   |
|           | 2           | 3      | 0:00:00            | 0.109    |
|           | 3           | 5      | 0:00:00            | 0.0700   |
|           | 4           | 2      | 0:00:00            | 0.971    |
|           | 5           | 8      | 0:00:00            | 0.00142  |
| Problem 2 |             |        |                    |          |
| Standard  | 1           | 296    | 0:00:02            | 0.000244 |
|           | 2           | 1,000  | 0:00:04            | 0.00334  |
|           | 3           | 69     | 0:00:00            | 0.000183 |
|           | 4           | 1,000  | 0:00:0             | 0.00219  |
|           | 5           | 1,000  | 0:00:05            | 0.000374 |
| New CG    | 1           | 20     | 0:00:00            | 0.0861   |
|           | 2           | 319    | 0:00:00            | 0.00291  |
|           | 3           | 36     | 0:00:00            | 0.00174  |
|           | 4           | 4      | 0:00:00            | 0.356    |
|           | 5           | 5      | 0:00:05            | 0.0937   |

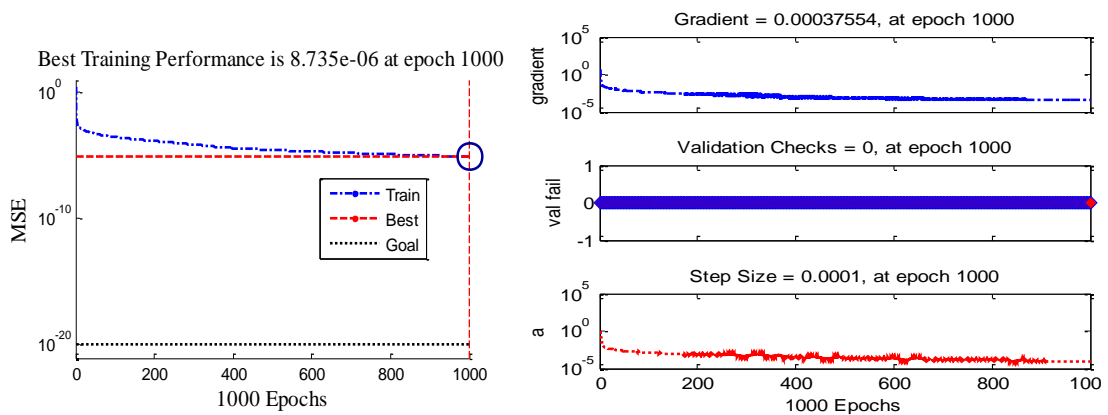


Figure 1. Performance of HS method for training neural networks using problem 1

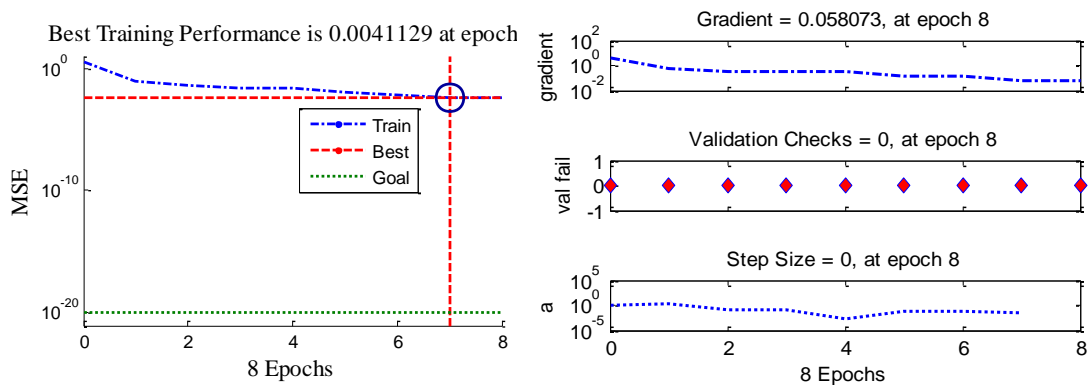


Figure 2. Performance of new method for training neural networks using problem 1

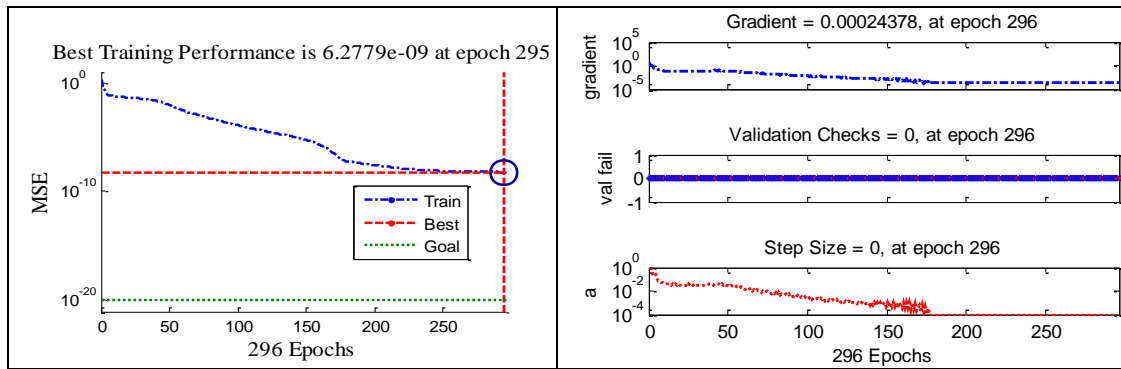


Figure 3. Performance of HS for training neural networks using problem 2

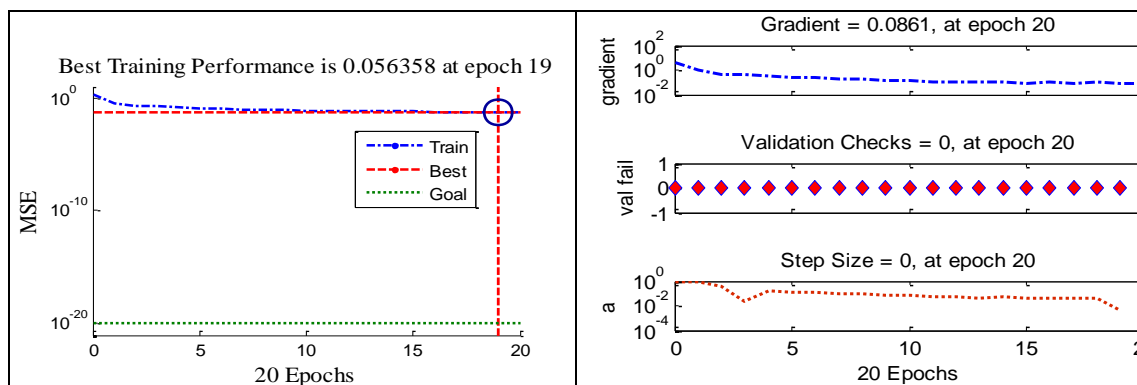


Figure 4. Performance of new method for training neural networks using problem 2

### 5. CONCLUSION

ANN has employed modified conjugate gradients since the 1980s with a variety of CG algorithms, including single modified and combinations of numerous CG techniques, according to preliminary study. The majority of the research was on increasing the effectiveness of learning algorithms during training. By using appropriate formulations and methods to improve the performance of all test data, this major objective will be accomplished. In addition, the review uses CG as a key component for fixing mistakes in the back-propagation process. In this paper, we presented a new CG method parameter based on the Perry parameter and a modified vector  $v_k^*$  based on the Barzilai and Borwein step size. The descent and sufficient descent requirements of the new method are established. Additionally, we investigate the global convergent property under accepted premises. The new method is more effective than the HS algorithm, as demonstrated by the numerical results on problems with low and high dimensionality. Finally, the new method's practical relevance for training neural networks is also investigated. When compared to some well-known algorithms, the strategy is utilized to increase the efficiency of neural networks.





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## BIOGRAPHIES OF AUTHORS



**Alaa Luqman Ibrahim**     is a teaching lecturer at the University of Zakho. He received a bachelor's degree in mathematics science from Duhok University and a master's degree in optimization from Zakho University. His current fields of interest area is Applied Mathematics and solve optimization models numerically and analytically in different fields. He can be contacted at email: [alaa.ibrahim@uoz.edu.krd](mailto:alaa.ibrahim@uoz.edu.krd).



**Mohammed Guhdar Mohammed**     is a teaching lecturer assistant at the University of Zakho. He received a bachelor's degree in computer science and a master's degree in artificial intelligence from Dohuk University. His current fields of interest are machine learning, algebra, bioinformatics, and computer vision. He can be contacted at email: [mohammed.guhdar@uoz.edu.krd](mailto:mohammed.guhdar@uoz.edu.krd).