Generalized Dai-Yuan conjugate gradient algorithm for training multi-layer feed-forward neural networks

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ABSTRACT
In this paper, we will present different type of CG algorithms depending on Peary conjugacy condition. The new conjugate gradient training (GDY) algorithm using to train MFNNs and prove it's descent property and global convergence for it and then we tested the behavior of this algorithm in the training of artificial neural networks and compared it with known algorithms in this field through two types of issues.
connection weights and other parameters in the algorithm such as momentum and the learning rate. The improving of the training efficiency of a NNs run large area of papers and several research have been introduced in the literature[4]. Bishop in [1] recapitulated several optimization techniques were proposed to improve the activity of learning efficiency i.e. the error minimization manner. Among these optimization algorithms[5], the non-linear conjugate gradient (CG) method, which is generated sequence of weights \{w_k\}_{k=1}^{\infty} with initial weights \( w_0 \in \mathbb{R}^n \). Firstly set \( d_0 = -g_0 \) and then a sequence \( w_k \) of the approximations to minimize is defined in the way:

\[ w_{k+1} = w_k + \alpha_k d_k, \quad k = 1,2,... \quad (3) \]

\[ d_{k+1} = -g_{k+1} + \beta_k d_k \quad (4) \]

The conjugate gradient algorithms have various types according to the way of predifining the parameter \( \beta_k \). As we known there has been suggested several selections for \( \beta_k \) which belongs to different conjugate gradient ways.

\[ \beta^{PE} = \frac{s_k^T g_{k+1}}{s_k^T g_k} \quad [6] \]

\[ \beta^{PR} = \frac{s_k^T g_{k+1}}{g_k^T s_k} \quad [7] \]

\[ \beta^{RO} = \frac{g_k^T s_{k+1}}{g_k^T s_k} \quad [8] \]

\[ \beta^{NS} = \frac{s_k^T g_{k+1}}{g_k^T s_k} \quad [9] \]

where \( y_k = g_{k+1} - g_k \). Often, to analysis the convergence of CG algorithms needs the inexact line search such as the standard Wolfe line search which defined by:

\[ F(w_k + \alpha_k d_k) \leq F(w_k) + \rho \alpha_k g_k^T d_k \quad (5) \]

\[ g(w_k + \alpha_k d_k)^T d_k \geq \sigma g_k^T d_k \quad (6) \]

While the strong condition of Wolfe line search are:

\[ F(w_k + \alpha_k d_k) \leq F(w_k) + \rho \alpha_k g_k^T d_k \]

\[ |g_{k+1}^T d_k| \leq \sigma | g_k^T d_k | \quad (8) \]

If \( 0 < \rho < \sigma < 1 \). Other consequential subject in the CG methods is the search directions produced by equation (4) are conjugate directions if the line search is exact and the objective function is convex that is:

\[ d_i^T G d_j = 0, \quad i \neq j \quad (9) \]

The variable \( G \) is devoted to the Hessian matrix of the objective function, it’s clear that the equation (9) can be rewritten in the following form:

\[ d_i^T y_j = 0 \quad (10) \]

which is called pure conjugacy condition. Perry in [10] generalized the conjugacy condition (10) for non-quadratic functions to the:

\[ d_i^T y_j = s_i^T y_j \quad (11) \]

where \( s_j = w_k + \alpha_k d_k \). Dai and Liao in [11] showed that for general objective function with inexact line search the equation (11) can be written as follows:

\[ d_i^T y_j = -s_i^T s_j, \quad \xi > 0 \quad (12) \]

This paper is planned as follows: In section 2, the novel conjugate gradient teaching (GDY) algorithm for MFNNs presented. Section 3 presents the descent property and global convergence for the proposed algorithm, while section 4 include the experimental results to appraisal the performance of the proposition training method and paragons it with famous training methods.

2. Derivation of the New GDY method

An advantage of Dai-Yuan method(\( \beta^{RO} \)) is that it ensures the direction is descent and hence the global convergence is achieved when implemented with the conditions of Wolfe line search. In the other hand the \( \beta^{PR} \) method has drawback similar to the \( \beta^{RO} \) method, so it cannot get out the cycles of the teeny steps, to overcome to this drawback, I suggest a new formula \( \beta^{NS} \) as follows: Consider the following search direction:

\[ d_{k+1} = -g_{k+1} + \left[ \frac{s_k^T g_{k+1}}{s_k^T y_k} \right] y_k \quad (13) \]

Now to find the value of \( \gamma \), multiply both side of equation (13) by \( y_k^T \) to get:

\[ y_k^T d_{k+1} = -y_k^T g_{k+1} + \left[ \frac{g_k^T s_{k+1}}{s_k^T y_k} \right] y_k^T s_k \quad (14) \]

From the equation (14) and Perr conjugacy condition (11) we get:

\[ -y_k^T g_{k+1} + y_k^T g_{k+1} - y_k^T g_{k+1} = -y_k^T g_{k+1} \]

\[ \Rightarrow y_k^T g_{k+1} = y_k^T g_{k+1} - (g_k^T s_k + g_k^T s_k) + s_k^T s_k \]

Therefore the value of \( \gamma \) is:

\[ \gamma = 1 + \frac{g_k^T s_k}{s_k^T s_k} \quad (15) \]

Substitute equation (15) in (13) to get:

\[ d_{k+1} = -g_{k+1} + \left[ \frac{g_k^T s_k}{s_k^T s_k} \right] y_k \quad (16) \]

Or \( \vdash d_{k+1} = -g_{k+1} + \beta_k s_k \quad (17) \)

At this point, we present a high level description of the proposed (GDY) algorithm:

The Algorithm(GDY)

Step0: Initiate \( w_1 \), and choose \( \sigma, \rho \) such that \( 0 < \rho < \sigma < 1 \),

\[ E_0, \varepsilon \leq 10^{-5} \& K_{max} \text{ set } k = 1. \]

Step 1: Compute \( E_k \) & \( g_k \) (i.e. the error function value and its gradient).

Step 2: IF \( |g_k| < \varepsilon or (E_k < E_0) \), set \( w_{opt} = w_k \) and \( E_{opt} = E_k \), print the goal is meet then stop .

Step 3: Calculate the descent direction: \( d_k = -g_k \) when \( k = 1 \) then go to

Step 5: Else \( d_{k+1} = -g_{k+1} + \beta_k s_k \).

Step 4: Calculate \( \alpha_k \) (the learning rate) using the standard conditions of Wolfe (5) and (6).

Step 5: Updating weights: \( w_k = w_k + \alpha_k d_k \)
and put \( k = k + 1 \).

Step 6: Stop if \( k > k_{\text{max}} \) and print the Error goal not reach, otherwise return to step 1.

3. Convergence analysis

The descent condition outplays an chief role in the global convergence analysis to many methods. The next theorem signifies that the algorithm (GDY) is produced a descent directions.

**Theorem (1)**
Consider the search directions generated by the equation (16) and assume that the learning rate \( \alpha_k \) satisfies the Wolfe condition (5) and (6), then \( d_k^T g_k < 0 \quad \forall k \geq 1 \)

**Proof:**
Clearly the theorem is true when \( k = 1 \), and suppose the theorem is true at \( k \), we shall show it is true at \( k = k + 1 \). Consider the search direction defined by equation (16)

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

Multiply both sides of the above equation by \( g_{k+1} \) to get:

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

\[
= -\left[ g_{k+1} \right]^{2} + \left[ g_{k+1}^T, g_k - g_{k+1}^T, s_k \right] \left[ s_k \right] g_{k+1}
\]

\[
= -\left[ g_{k+1} \right]^{2} + \left[ g_{k+1}^T, y_k - g_{k+1}^T, s_k \right] \left[ s_k \right] g_{k+1}
\]

use Lipschitz condition with \( 0 < L \leq 1 \) and \( y_k^T s_k > 0 \)

To get

\[
d_{k+1}^T g_{k+1} \leq -\left[ g_{k+1} \right]^{2} + \left( L - 1 \right) \left( y_k^T s_k \right) < 0
\]

Toward analyze the globally convergence property of the proposed algorithm (GDY), the next assumption are required. These assumptions have been used extensively in the literature for the global convergence analysis of conjugate gradient methods.

**Assumption H**
1- Let set \( \psi = \{ w \in R^n | E(w) \leq E(w) \} \) then the level \( \psi \) is bounded, that is, \( \exists \) a constant \( B > 0 \) satisfying:

\[ |w| \leq B \quad \text{for all} \ w \in N \] (18)

2- Suppose that \( f \) is continuously differentiable function and its gradient is Lipschitz continuous in some neighborhood \( N \) of \( \psi \), i.e. \( \exists \) a positive \( L \) such that:

\[ |g(w) - g(w_2)| \leq L |w - w_2|, \forall w, w_2 \in N \] (19)

Obviously, Assumption H denotes that \( \exists \) a scaler \( \gamma \) such that:

\[ |g(w)| \leq \gamma \quad \forall w \in N \] (20)

Now, we can obtain the next general result to any CG method satisfied strong Wolfe line search, which is attained in [1].

**Lemma (1)**
Assume that Assumption H satisfies. Consider a CG method in the form (3)-(17) such that \( \alpha_k \) is computed from the strong Wolfe line search and \( d_k \) is a descent direction, if:

\[ \sum_{i=1}^{k} \left[ d_i \right] = \infty \] (21)

we have that:

\[ \lim_{k \to \infty} \text{inf} \left[ g_k \right] = 0 \] (22)

For any uniformly convex function, we can verify that \( |d_k| \) which generated by (17) is restricted from above. Therefore by using Lemma (1) we get the next result.

**Theorem (2)**
Assume that Assumption H is hold. Consider the direction search (16), where \( d_k \) is satisfied descent condition (i.e. \( g_k^T d_k < 0 \) and \( \alpha_k \) is computed using strong Wolfe line search). If \( \exists \) constant \( \mu > 0 \) satisfying:

\[ (\forall z) - \text{Wolfe line search} \] (23)

We have:

\[ \lim_{k \to \infty} \left[ g_k \right] = 0 \] (24)

**Proof:**
We will demonstrate this theory using the method of contradiction, take the norm to the equation (17) to get:

\[ |\beta| = \left[ \left[ g_k \right] \right] - \left[ s_k \right] g_{k+1} \left[ s_k \right] g_{k+1} \] (25)

Since \( s_k y_k > 0 \) by Wolfe condition then:

\[ |\beta| \leq \left[ g_k \right] \frac{y_k}{s_k y_k} \frac{g_k}{s_k y_k} + \left[ g_k \right] \frac{y_k}{s_k y_k} \] (26)

Now, to both sides of equation (16) take the norm to get:

\[ |d_k| = \left[ \left[ g_k \right] \right] - \beta \Rightarrow |d_k| \leq \left[ g_k \right] + |\beta| \left[ x_k \right] \] (27)

And offset the equation (26) in (27) get:

\[ |d_k| \leq \left[ g_k \right] \frac{y_k}{s_k y_k} + \left[ g_k \right] \frac{y_k}{s_k y_k} + \left[ g_k \right] \frac{y_k}{s_k y_k} \] (28)

Substitute equation (20) in (28) to get:

\[ |d_k| \leq \gamma \frac{y_k}{s_k y_k} + \left[ x_k \right] \frac{y_k}{s_k y_k} + \left[ x_k \right] \frac{y_k}{s_k y_k} \] (29)

By using equation (23) for \( W_k \) and \( W_{k+1} \) we have:

\[ s_k y_k \leq \left[ x_k \right] \frac{y_k}{s_k y_k} \] (30)

Therefore (29) become:

\[ |d_k| \leq \gamma \left[ \frac{r_k}{\ll d_k, l_k} \right] + \left[ x_k \right] \frac{y_k}{s_k y_k} + \left[ x_k \right] \frac{y_k}{s_k y_k} \] (31)

Suppose that there exist constants \( n_1, n_2 \) and \( n_3 \) such that:

\[ n_1 = (\gamma + \frac{r_k}{L}) \quad \text{and} \quad n_2 = \frac{y_k}{L} \] (32)

written as:

\[ |d_k| \leq n_1 + n_2 = n_3 \] (33)
\[ \frac{1}{\|v_{k}\|^2} \geq \frac{1}{\|v_{k-1}\|^2} \geq \frac{1}{\|v_{0}\|^2} \implies \sum_{k} \frac{1}{\|v_{k}\|^2} > \sum_{k} \frac{1}{\|v_{0}\|^2} > -\infty \]

This is a contradiction lemma (1)

\[ \sum_{k} \frac{1}{\|v_{k}\|^2} = \infty \implies \lim_{k \to \infty} \|g_{k}\| = 0 \]

4. The experiments Results:

In this part of the search, we will study the results of numerical experimental to show the activity of the proposed in three problems the Monk1-problem, Monk2-problem and continuous function approximation problem. A comparison was made between the performance of the proposed algorithm (GDY) with offline versions of the conjugate gradient method and each algorithm Fletcher_Reeves update (FRCG) which is known as (traincgf) and Polack_Ribiere method (PRCG) update which is denoted by (traincgp) (see appendix of MATLAB) as well as Dia-Yuan whose program code was written for not otherwise available in the toolboxes of MATLAB.

The simulation was performed using MATLAB (2009a). The same random weights for each algorithm were used during the comparison process and generated them using the Nguyen-Widrow method [12]. It is worth noting that the default values of the parameters and the explanatory tools for the algorithms mentioned above were used unless otherwise stated. For all the three test questions mentioned above we was written the summarise of the performance to each algorithm for 100 simulations as table that reached a solution within a predetermined limit of time. The parameters used in all tables are: timemean the average of total time; epochmean average of total numbers of epochs, perfmean average of total perform, gradient, the mean value of the gradient, and Succ is denoted to the succeeded simulations out of (100) marks within error function evaluations limit. All methods have been implemented with the Wolfe line search conditions (5) and (6).

Finally, It is worth mentioning that it has been considered that the algorithm has failed to train the artificial neural network if it does not reach the solution within the predetermined number of parameters and thus its epoch are not enter the statistical analysis of the algorithm.

4.1 Monk's Problems

Monk's problems are one of the first problems used to compare the performance of different learning algorithms of the neural network. This data consists of three binary classification problems based on the artificial robot domain, which are described by six different binary features. Symbolic rules There are three problems in Monk. The domains for all Monk problems are the same (432 patterns). The domain of each problem has been separated into a test and train set[12]:

4.1.1 MONK-1 contains 124 examples chosen randomly from the data group used it to train the network and the remaining data(308 examples) were applied to test the network (table(1)) and the figure (1) illustrates the behavior of these algorithms. We note from the table(1) that the proposed method approaches the behavior of the PRCG while there is a significant difference between it and the FRCG.

4.1.2 MONK-2 includes 169 patterns selected at randomly from the data group to train so the residual 263 patterns used to test the network (table(2)) while the figure (2) shows the path of convergence of these algorithms to the desired error value which is (1*10^-10).

4.2 Continuous Function Approximation:

The approximation function of the continuous trigonometric function which can be written as:

\[ f(w) = \cos(3w) * \sin(w) \]

is considered as one of the known issues for training neural networks.

The artificial neural network architecture used to solve this problem consists of a single neuron in both the input and output layer, as well as a hidden layer, which is the middle of the input and output layer consist of fifteen neurons equipped with 30 weights and 16 biases. The network is learned who to approximate the function \( f(w) \cdot w \in [-\pi, \pi] \) and stopped when sum of squares of the errors come to be fewer than 0.001 (the goal). The hidden neurons of network used the logistic function as activation function and the linear activations function in the output layer. The convergence of these algorithms from the target is shown in Figure (3) and the comparative results are shown in table (3) Which shows us a close convergence in the behavior of the functions PRCG and the new algorithm DGY.
Results of Simulations for the Continuous Fun. Approx.Problem table(3)

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>timemean</th>
<th>Epochmean</th>
<th>Perfmean</th>
<th>Gradient</th>
<th>Succ</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRCG</td>
<td>3.5358</td>
<td>119.24</td>
<td>0.0019505</td>
<td>0.020778</td>
<td>%100</td>
</tr>
<tr>
<td>FRCG</td>
<td>5.4828</td>
<td>216.84</td>
<td>0.0019717</td>
<td>0.038426</td>
<td>%100</td>
</tr>
<tr>
<td>DYCG</td>
<td>3.5594</td>
<td>113</td>
<td>0.0019549</td>
<td>0.02394</td>
<td>%100</td>
</tr>
<tr>
<td>GDY</td>
<td>3.6736</td>
<td>118.72</td>
<td>0.0019486</td>
<td>0.020128</td>
<td>%100</td>
</tr>
</tbody>
</table>

**Conclusion**

In this search, we proposed a new conjugate gradient method can be used it to train feed forward neural networks with multilayer, the derivation of the value of $\beta_k$ is based on Peary conjugacy condition. The proposed method holds descent and globally convergence under the standard Wolfe conditions. Practically, the numerical experiments showed that the convergent behavior of the proposed algorithm GDY with the Polack Ribiere method and the large variation between it and the functions FRCG and DYCG in the other hand.

**References**


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