

A Framework for the Development of Globally Convergent Adaptive Learning Rate Algorithms

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Abstract: In this paper we propose a framework for developing globally convergent batch training algorithms with adaptive learning rate. The proposed framework provides conditions under which global convergence is guaranteed for adaptive learning rate training algorithms. To this end, the learning rate is appropriately tuned along the given descent direction. Providing conditions regarding the search direction and the corresponding stepsize length this framework can also guarantee global convergence for training algorithms that use a different learning rate for each weight. To illustrate the effectiveness of the proposed approach on various training algorithms simulation results are provided.

Keywords and phrases: Global convergence, learning rate adaptation, batch training algorithms, steepest descent, feedforward neural networks.

1. Introduction

Supervised neural network training is a subject of considerable ongoing research and numerous algorithms have been proposed to this end. A common approach is to realize training by minimizing the network learning error, which is a measure of its performance and is usually based on the difference between the actual output vector of the network and the desired output vector. The rapid computation of a set of weights that minimizes this error is a rather difficult task since, in general, the number of network weights is high and the error function generates a complicated surface in the weight space, possessing multitudes of local minima and having broad flat regions adjoined with narrow steep ones that need to be searched to locate an "optimal" weight set.

In order to simplify the formulation of the equations throughout the paper a unified notation for the weights is adopted. Thus, for a Feedforward Neural Network (FNN) with a total of n weights, \mathbb{R}^n is the n -dimensional real space of column weight vectors w with components w_1, w_2, \dots, w_n and w^* is the optimal weight vector with components $w_1^*, w_2^*, \dots, w_n^*$; E is the batch error measure defined as the sum-of-squared-differences error function over the entire training set; $\partial_i E(w)$ denotes the partial derivative of $E(w)$ with respect to the i th variable w_i ; $\nabla E(w)$ defines the gradient vector of the sum-of-squared-differences error function E at w while $H = [H_{ij}]$ defines the Hessian $\nabla^2 E(w)$ of E at w .

The special case of the batch training is consistent with the theory of unconstrained optimization. In this case the minimization corresponds to updating the weights after each presentation of the entire training set, which is called an *epoch*, and requires that the sequence of weight vectors $\{w^k\}_{k=0}^{\infty}$, where k indicates epochs, converges to a set w^* that minimizes E .

The widely used batch Back-Propagation (BP) [23] is a first-order training algorithm, which minimizes the error function using the steepest descent method [8]:

$$w^{k+1} = w^k - \eta \nabla E(w^k), \quad (1)$$

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where the gradient vector is usually computed by the back-propagation of the error through the layers of the FNN (see [23]) and η is a heuristically chosen constant parameter, called learning rate. Appropriate learning rates help to avoid convergence to a saddle or maximum point. In practice, a small constant learning rate is chosen ($0 < \eta < 1$) in order to secure the convergence of the BP algorithm and to avoid oscillations in the directions where the error surface is steep. However, this approach considerably slows down the training process since, in general, a small learning rate may not be appropriate for all the portions of the error surface.

Our motivation in this paper is to provide general theoretical results and strategies that are applicable to guarantee the convergence of adaptive learning rate algorithms. The algorithms differ according to the information they need to modify the learning rate. In training algorithms with a *global* learning rate, the same rate is used to update all the weights in the FNN, while in algorithms with a *local* learning rate a different learning rate is used for each weight.

The paper is organized as follows. Section 2 provides an overview of adaptive learning rate BP algorithms. In Section 3 the issues of monotone decrease of the error function, as well as the notion of global convergence are introduced. Then, strategies for developing globally convergent modifications of adaptive learning rate algorithms are presented in Sections 4 and 5, while in Section 6 we present an application example to evaluate and compare various adaptive learning rate algorithms. Finally, the paper ends in Section 7 with some concluding remarks.

2. Adaptive learning rate algorithms

Several adaptive learning rate algorithms have been proposed to accelerate the training procedure. The following strategies are usually suggested:

- (i) start with a small learning rate and increase it exponentially if successive epochs reduce the error, or rapidly decrease it if a significant error increase occurs [2, 25],
- (ii) start with a small learning rate and increase it if successive epochs keep gradient direction fairly constant, or rapidly decrease it if the direction of the gradient varies greatly at each epoch [4] or
- (iii) for each weight an individual learning rate is given, which increases if the successive changes in the weights are in the same direction and decreases otherwise [10, 19, 21, 24].

Note that all the above mentioned strategies employ heuristic parameters in an attempt to enforce the monotone decrease of the learning error and to secure the converge of the training algorithm to a minimizer of E .

A different approach is based on Goldstein's and Armijo's work on steepest-descent and gradient methods. The method of Goldstein [9] requires the assumption that E is twice continuously differentiable on $\mathcal{S}(w^0)$, where $\mathcal{S}(w^0) = \{w : E(w) \leq E(w^0)\}$ is bounded, for some initial vector w^0 . It also requires that η is chosen to satisfy the relation $\sup \|H(w)\| \leq \eta^{-1} < \infty$ in some bounded region, where the relation $E(w) \leq E(w^0)$ holds. The k th iteration of an algorithm model that follows this approach consists of the following steps:

1. Choose η_0 to satisfy $\sup \|H(w)\| \leq \eta_0^{-1} < \infty$ and δ to satisfy $0 < \delta \leq \eta_0$.
2. Set $\eta^k = \eta$, where η is such that $\delta \leq \eta \leq (2\eta_0 - \delta)$ and go to the next step.
3. Update the weights $w^{k+1} = w^k - \eta^k \nabla E(w^k)$.

However, the manipulation of the full Hessian is too expensive in computation and storage for FNNs with several hundred weights [3]. Le Cun [11] proposed a technique, based on appropriate perturbations of the weights, for estimating on-line the principle eigenvalues and eigenvectors of the Hessian without

calculating the full matrix H . According to experiments reported in [11] the largest eigenvalue of the Hessian is mainly determined by the FNN architecture, the initial weights and by short-term low-order statistics of the training data. This technique could be used to determine η_0 , in Step 1 of the above algorithm, requiring additional presentations of the training set in the early training.

An alternative approach is based on the work of Armijo [1]. Following this approach, the value of the learning rate η is related to the value of the Lipschitz constant K , which depends on the morphology of the error surface. In this case, the BP algorithm takes the form:

$$w^{k+1} = w^k - \frac{1}{2K} \nabla E(w^k), \quad (2)$$

and converges to the point w^* which minimizes E (see [1] for conditions under which convergence occurs and a convergence proof). However, in practice neither the morphology of the error surface nor the value of K are known a priori. In [13] a local estimation of the Lipschitz constant has been proposed, as part of a learning rate adaptation strategy that provides increased rate of convergence through the Lipschitz constant estimation and guarantees the stability of the learning procedure.

3. Monotone decrease of the error function and global convergence

A training algorithm can be made globally convergent by determining the learning rate in such a way that the error is exactly minimized along the current search direction at each epoch, i.e. $E(w^{k+1}) < E(w^k)$. To this end, an iterative search, which is often expensive in terms of error function evaluations, is required. It must be noted that the above simple condition does not guarantee global convergence for general functions, i.e. converges to a local minimizer from any initial condition (see [5] for a general discussion on globally convergent methods).

The use of adaptive learning rate algorithms which enforce monotonic error reduction using inappropriate values for the critical heuristic learning parameters can considerably slow the rate of training, or even lead to divergence and to premature saturation [12, 22]. Moreover, using heuristics it is not possible to develop globally convergent training algorithms.

To alleviate this situation it is preferable to tune the learning rate, which is evaluated by an adaptive learning rate algorithm, so that the value of the error function is sufficiently decreased at each epoch, accompanied by a significant change in the value of w . A strategy of this kind consists in accepting a positive learning rate η^k along the search direction φ^k if it satisfies the *Wolfe conditions*:

$$E(w^k + \eta^k \varphi^k) - E(w^k) \leq \sigma_1 \eta^k \langle \nabla E(w^k), \varphi^k \rangle, \quad (3)$$

$$\langle \nabla E(w^k + \eta^k \varphi^k), \varphi^k \rangle \geq \sigma_2 \langle \nabla E(w^k), \varphi^k \rangle, \quad (4)$$

where $0 < \sigma_1 < \sigma_2 < 1$ and $\langle \cdot, \cdot \rangle$ stands for the usual inner product in \mathbb{R}^n . The first inequality ensures that the error is reduced sufficiently and the second prevents the learning rate from becoming too small. It can be shown that if φ^k is a descent direction, if E is continuously differentiable and if E is bounded below along the radius $\{w^k + \eta \varphi^k \mid \eta > 0\}$, then there always exist learning rate satisfying (3)-(4) [5, 16]. Relation (4) can be replaced by [5]:

$$E(w^k + \eta^k \varphi^k) - E(w^k) \geq \sigma_2 \eta^k \langle \nabla E(w^k), \varphi^k \rangle, \quad \sigma_2 \in (\sigma_1, 1). \quad (5)$$

An alternative strategy has been proposed in [20]. It is applicable to any descent direction φ^k and uses two parameters $\alpha, \beta \in (0, 1)$. Following this approach the learning rate is $\eta^k = \beta^{m_k}$, where $m_k \in \mathbb{Z}$ is any integer such that:

$$E(w^k + \beta^{m_k} \varphi^k) - E(w^k) \leq \beta^{m_k} \alpha \langle \nabla E(w^k), \varphi^k \rangle, \quad (6)$$

$$E(w^k + \beta^{m_k-1} \varphi^k) - E(w^k) > \beta^{m_k-1} \alpha \langle \nabla E(w^k), \varphi^k \rangle. \quad (7)$$

An algorithm model that incorporates the above strategy is given below.

Algorithm 1

1. **Input** $\{E; w^0; \alpha, \beta \in (0, 1); m^* \in \mathbb{Z}; MIT; \varepsilon\}$.
2. **Set** $k = 0$.
3. **If** $\|\nabla E(w^k)\| \leq \varepsilon$ **go to** Step 6. **Else**, compute a descent direction φ^k .
4. **compute** the learning rate $\eta^k = \beta^{m_k}$, where $m_k \in \mathbb{Z}$ is any integer such that
 - (a) $E(w^k + \beta^{m_k} \varphi^k) - E(w^k) \leq \beta^{m_k} \alpha \langle \nabla E(w^k), \varphi^k \rangle$ and
 - (b) $E(w^k + \beta^{m_k-1} \varphi^k) - E(w^k) > \beta^{m_k-1} \alpha \langle \nabla E(w^k), \varphi^k \rangle$.
5. **Set** $w^{k+1} = w^k + \eta^k \varphi^k$. **If** $k < MIT$, replace k by $k + 1$, and **go to** Step 3; **otherwise go to** Step 6.
6. **Output** $\{w^k; E(w^k); \nabla E(w^k)\}$.

For an extended version of Algorithm 1, see [26]. All the above strategies must be combined with tuning subprocedures generating learning rates that satisfy conditions (3)–(4) or (6)–(7) in order to guarantee global convergence. This issue is the subject of the next section.

4. Global convergence by tuning the learning rate

In this section we propose learning rate tuning subprocedures and establish useful convergence theorems due to Wolfe [27, 28] and Polak [20]. The strategy based on Wolfe's conditions provides an efficient and effective way to ensure that the error function is globally reduced sufficiently. In practice, the conditions (4) and (5) are generally not needed because the use of a backtracking strategy avoids very small learning rates. A simple backtracking strategy to tune the length of the minimization step, so that it satisfies conditions (3)–(4) at each epoch, is to decrease the learning rate by a reduction factor $1/q$, where $q > 1$ [17]. This has the effect that the learning rate is decreased by the largest number in the sequence $\{q^{-m}\}_{m=1}^{\infty}$, so that the condition (3) is satisfied. We remark here that the selection of q is not critical for successful learning, however it has an influence on the number of error function evaluations required to satisfy the condition (3). Thus, when seeking to satisfy (3) it is important to ensure that the learning rate is not reduced unnecessarily so much that the condition (4) is not satisfied. Since in training the gradient vector is known only at the beginning of the iterative search for a new weight vector, the condition (4) cannot be checked directly (this task requires additional gradient evaluations at each epoch), but is enforced simply by placing a lower bound on the acceptable values of the learning rate. This bound on the learning rate has the same theoretical effect as the condition (4) and ensures global convergence [5]. The value $q = 2$ is usually suggested in the literature [1] and indeed it was found to work without problems in the experiments (see [14]).

In this framework, an important theorem due to Wolfe [5] states that if E is bounded below, then the sequence $\{w^k\}_{k=0}^{\infty}$ generated by any algorithm that follows a descent direction φ^k whose angle θ_k with $-\nabla E(w^k)$ is such that:

$$\cos \theta_k = \frac{\langle -\nabla E(w^k), \varphi^k \rangle}{\|\nabla E(w^k)\| \|\varphi^k\|} > 0, \quad (8)$$

and satisfy the Wolfe's conditions, will also obey $\lim_{k \rightarrow \infty} \nabla f(w^k) = 0$ [5, 16].

Theorem 1 [5, 16, 27, 28]. *Suppose that the error function $E : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuously differentiable on \mathbb{R}^n and assume that ∇E is Lipschitz continuous on \mathbb{R}^n . Then, given any $w^0 \in \mathbb{R}^n$, either E is unbounded below, or there exists a sequence $\{w^k\}_{k=0}^{\infty}$ obeying the Wolfe's conditions (3)–(4) and either:*

- (1) $\langle \nabla E(w^k), (w^{k+1} - w^k) \rangle < 0$, or
 (2) $\nabla E(w^k) = 0$, and $w^{k+1} - w^k = 0$,

for each $k > 0$. Furthermore, for any such sequence, either:

- (a) $\nabla E(w) \neq 0$ for some $k \geq 0$, or
 (b) $\lim_{k \rightarrow \infty} E(w^k) = -\infty$, or
 (c) $\lim_{k \rightarrow \infty} \langle \nabla E(w^k), (w^{k+1} - w^k) \rangle / \|w^{k+1} - w^k\| = 0$.

This is also true when Relation (4) is replaced by Relation (5) [5] (cf. Relation (b) of Step 4 of Algorithm 1). For a relative convergence result where the sequence $\{w^k\}_{k=0}^{\infty}$ converges q -superlinearly to a minimizer w^* see [5].

Regarding Polak's approach, if the error function E is bounded from below the following subprocedure can be used to find an m_k satisfying Relations (a) and (b) of Step 4 of the Algorithm 1. This subprocedure uses the last used learning rate $\eta^{k-1} = \beta^{m_{k-1}}$ as the starting point for the computation of the next one [20]:

1. If $k = 0$, set $m' = m^*$. Else set $m' = m_{k-1}$.
2. If $m_k = m'$ satisfies Relations (a) and (b) of Step 4 of Algorithm 1, stop.
3. If $m_k = m'$ satisfies (a) but not (b), replace m' by $m' - 1$, and go to Step 2.
 If $m_k = m'$ satisfies (b) but not (a), replace m' by $m' + 1$, and go to Step 2.

In practice, only a very small number of iterations of the above subprocedure is required to compute the learning rate. The search strategy of Algorithm 1 allows us to establish the following useful convergence theorem due to Polak [20]: This theorem requires the search direction φ^k to be bounded from above, it imposes a restriction on the angle between $\nabla E(w^k)$ and φ^k (see Relation (8)), and states that Algorithm 1 is well defined in the sense that whenever $\nabla E(w^k) \neq 0$, the search for a learning rate η^k is a finite process.

Theorem 2 [20]. Assume that (i) the error function $E : \mathbb{R}^n \rightarrow \mathbb{R}$ is Lipschitz continuously differentiable on bounded sets; (ii) the sequences $\{w^k\}_{k=0}^{\infty}$ and $\{\varphi^k\}_{k=0}^{\infty}$ are constructed by Algorithm 1; (iii) there exist two continuous functions $N_1 : \mathbb{R}^n \rightarrow \mathbb{R}$ and $N_2 : \mathbb{R}^n \rightarrow \mathbb{R}$ such that:

- (1) for all w satisfying $\nabla E(w) \neq 0$, $N_1(w) > 0$, $N_2(w) > 0$ and $N_1(w) = 0$ if and only if $\nabla E(w) = 0$ and
- (2) for all $k \in \mathbb{N}$, the w^k and φ^k satisfy the inequalities $\langle \nabla E(w^k), \varphi(w^k) \rangle \leq -N_1(w^k)$, and $\|\varphi^k\| \leq N_2(w^k)$.

Under these assumptions,

- (a) if w^k is such that $\nabla E(w^k) \neq 0$, then η^k is computed by Algorithm 1 using a finite number of function evaluations and
- (b) any accumulation point w^* of the sequence $\{w^k\}_{k=0}^{\infty}$ satisfies $\nabla E(w^*) = 0$.

5. Global convergence by adapting the search direction

A batch BP algorithm with a different learning rate for each weight is defined by the iterative scheme:

$$w^{k+1} = w^k - \text{diag}\{\eta_1^k, \eta_2^k, \dots, \eta_n^k\} \nabla E(w^k). \quad (9)$$

The learning rates are evaluated employing heuristic procedures that exploit information regarding the history of the partial derivative of $E(w)$ with respect to the i th weight and/or, depending on the algorithm, the history of the corresponding learning rate. Appropriate values of the heuristics ensure that the error function is decreased in each weight direction, every epoch. The well known *delta-bar-delta* method [10] and Silva and Almeida's method [24] follow this approach. Another method, named *quickprop* [6] is based on independent secant steps in the direction of each weight. The *Rprop* algorithm [21] updates the weights using the learning rate and the sign of the partial derivative of the error function with respect to each weight.

Clearly, the weight vector in Eq. (9) is not updated in the direction of the negative of the gradient; instead, an alternative adaptive search direction is obtained by taking into consideration the weight change, evaluated by multiplying the length of the search step, i.e. the value of the learning rate, along each weight direction by the partial derivative of $E(w)$ with respect to the corresponding weight, i.e. $-\eta_i \partial_i E(w)$. In other words, the algorithms of this class try to decrease the error in each direction, by searching the local minimum with small weight steps. These steps are usually constraint by problem-dependent heuristic parameters in order to ensure subminimization of the error function in each weight direction.

A well known difficulty of this approach is that the use of inappropriate heuristic values for a weight direction misguides the resultant search direction. In such cases, the training algorithm cannot exploit the global information obtained by taking into consideration all the directions. To alleviate this situation, we propose the search direction to be obtained by taking into consideration $n - 1$ learning rates, as directly evaluated by any adaptive learning rate algorithm and analytically evaluate the remaining one. This approach has the effect that the search direction is properly corrected and ensures that the direction followed is indeed a descent one. The following theorem provides a global convergence result for training algorithms with a different learning rate for each weight.

Theorem 3. *Suppose that the error function $E : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuously differentiable. Assume that ∇E is Lipschitz continuous on \mathbb{R}^n . Then, given any point $w^0 \in \mathbb{R}^n$, for any sequence $\{w^k\}_{k=0}^{\infty}$, generated by the iterative scheme:*

$$w^{k+1} = w^k - \tau^k \text{diag}\{\eta_1^k, \eta_2^k, \dots, \eta_n^k\} \nabla E(w^k), \quad (10)$$

where $\tau^k > 0$ satisfies the Wolfe's conditions (3)-(4) implies that

$$\lim_{k \rightarrow \infty} \nabla E(w^k) = 0.$$

Proof: Evidently, the error function E is bounded below on \mathbb{R}^n . The sequence $\{w^k\}_{k=0}^{\infty}$ follows the direction

$$\varphi^k(w^k) = -\text{diag}\{\eta_1^k, \eta_2^k, \dots, \eta_n^k\} \nabla E(w^k),$$

which is a descent direction when

$$\langle \nabla E(w^k), \varphi^k(w^k) \rangle < 0.$$

In that case, since E is continuously differentiable and bounded below there always exist τ^k satisfying the Wolfe's conditions:

$$E(w^k + \tau^k \varphi^k) - E(w^k) \leq \sigma_1 \tau^k \langle \nabla E(w^k), \varphi^k \rangle, \quad (11)$$

$$\langle \nabla E(w^k + \tau^k \varphi^k), \varphi^k \rangle \geq \sigma_2 \langle \nabla E(w^k), \varphi^k \rangle, \quad (12)$$

for $0 < \sigma_1 < \sigma_2 < 1$. Moreover, the restriction on the angle θ_k is fulfilled since for a descent direction φ^k it can be easily justified utilizing Relation (8) that $\cos \theta_k > 0$. Thus, by the Wolfe's Theorem [5], it holds that $\lim_{k \rightarrow \infty} \nabla E(w^k) = 0$. Thus the Theorem is proved.

Remark 1: Note that for neural networks with sigmoid activation functions the assumption of continuous differentiability of the error function is redundant.

Remark 2: A relative convergence result can be proved for any sequence $\{w^k\}_{k=0}^{\infty}$ satisfying the relations (3) and (5).

Remark 3: The use of $\tau^k = 1$ is suggested. This has the effect that the minimization step along the resultant search direction is defined by the value of the learning rates. By tuning τ^k , the length of the minimization step is regulated to satisfy the Wolfe's conditions, while the weights are updated in a descent direction.

6. Application example

The proposed strategies have been incorporated in various steepest descent-based and conjugate gradient-based training algorithms to develop new globally convergent modifications of these algorithms. These modified schemes have been implemented and tested on different training problems and have been compared in terms of epochs, gradient and error function evaluations and rate of success with other popular training methods. The results have been quite satisfactory. Our experience is that these strategies behave predictably and reliably. In this section we report an instance of our experimental study. More specifically we exhibit results on the numeric font learning problem [14, 26] for the following methods:

- (i) the batch Back-Propagation (BP) with a constant learning rate [23];
- (ii) the batch BP with adaptive learning rate [14] enhanced by the new strategy, which results in a BP training algorithm with inexact Line Search (BPLS) for the determination of a global learning rate;
- (iii) the BP with constant learning rate and Momentum (BPM) [23];
- (iv) the BP with Variable Stepsize (BPVS) [13];
- (v) the BP with Multi-learning Rate (BPMR), i.e a different adaptive learning rate for each weight [14], which incorporates the new strategy;
- (vi) the Fletcher-Reeves (FR) method [7];
- (vii) the Polak-Ribiere (PR) method [7];
- (viii) the Polak-Ribiere (PR) method constrained by the FR method (PR-FR) [7];
- (ix) the BP with heuristically determined adaptive learning rate and momentum proposed by Vogl et al. [25] (VMRZA);
- (x) the accelerated BP proposed by Parlos et al. [18] (PFAMT), which is now enhanced by the proposed strategy to avoid the jumpy behavior of the weights; and
- (xi) the Silva-Almeida (SA) method [24] that uses sign-based information to adapt local learning rates.

The algorithms testing has been conducted using the same 1000 initial weight vectors, which have been randomly chosen from a uniform distribution in the interval $(-1, 1)$.

In this application a 64-6-10 FNN (444 weights, 16 biases) is used for recognizing an 8×8 pixel machine printed numeral ranging from 0 to 9. The FNN is based on neurons of the logistic activation model.

Table 1: Results of Simulations for the Numeric Font Learning Problem

Algorithm	μ_{EP}	μ_{GFE}	Success
BP	14489	28978	660/1000
BPLS	12225	24454	990/1000
BPM	10142	20284	540/1000
BPVS	253	636	1000/1000
BPML	159	740	1000/1000
FR	620	3121	420/1000
PR	649	2124	960/1000
PR-FR	750	3473	1000/1000
VMRZA	1975	3950	910/1000
PFAMT	304	2419	1000/1000
SA	1400	2800	680/1000

The results exhibited in Table 1 are in terms of the average number of epochs (μ_{EP}) required to obtain a local minimum with batch error value $E \leq 10^{-3}$, the average number of the corresponding gradient and function evaluations (μ_{GFE}) and the number of successful runs out of 1000 (Success).

It is worth mentioning the difference that appears between the number of gradient evaluations and the number of error function evaluations at each epoch: in the BP, the BPM, the VMRZA and the SA, the batch error function and its gradient are evaluated only once, while there is a number of additional error function evaluations for all other algorithms tested when the Wolfe conditions are not fulfilled. For example, BPML needs an average of 159 epochs to converge, which corresponds to 740 gradient and error function evaluations, i.e to 159 gradient and 581 error function evaluations. However, note that in training practice a gradient evaluation is usually considered three times more costly than an error function evaluation [15]. By exhibiting this performance, BPML significantly outperforms the original method in the same example (see [14]).

7. Concluding remarks

A framework for the development of globally convergent batch training algorithms with adaptive learning rates has been proposed. The proposed framework provides conditions under which global convergence is guaranteed and strategies for tuning the adaptive learning rate and the search direction. A new general result for the global convergence has been established which is applicable to a class of training algorithm that use a different learning rate for each weight.

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