A Global Algorithm for Training Multilayer Neural Networks

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We present a global algorithm for training multilayer neural networks in this Letter. The algorithm is focused on controlling the local fields of neurons induced by the input of samples by random adaptations of the synaptic weights. Unlike the backpropagation algorithm, the networks may have discrete-state weights, and may apply either differentiable or nondifferentiable neural transfer functions. A two-layer network is trained as an example to separate a linearly inseparable set of samples into two categories, and its powerful generalization capacity is emphasized. The extension to more general cases is straightforward.

The multilayer neural network, trained by the backpropagation (BP) algorithm, is currently the most widely used neural network since it can solve linearly inseparable classification problems [1,2]. The BP algorithm is responsible for the rebirth of neural networks.

However, the BP algorithm has several limitations. Firstly, it requires the neural transfer functions to be differentiable in order to calculate the derivatives with respect to the synaptic weights. Secondly, the performance index to be minimized is constantly to be mean square error, because a non-quadratic performance index may result in a very complex performance surface. Finally, the synaptic weights obtained by this algorithm are continuous as a consequence of its updating equation of synaptic weights. These limitations are also inherent in variations of the BP algorithm. The last is indeed also a limitation for most of the learning rules for training single-layer neural networks. Discrete synaptic states have not only the advantage for digital hardware realization but also an experimental reality. Recent experiments have shown that the synaptic states in certain real neural network systems may be discrete [3–5].

The BP algorithm is a local learning rule. Most of the learning rules for training single-layer neural networks, such as the perceptron rule, the Hebb rule, and the Widrow-Hoff rule, are local rules. When training a network using a local rule, one inputs the samples into the network one by one, and each time the synaptic weights are updated independently on other samples. A step of update of synaptic weights induced by the input of a sample is an optimal solution for this sample, but not for other samples.

In principle, it is more favorable if each step of the update is an optimal solution for all the samples. This requires the consideration of the whole set of samples globally. An influential example of global rules is the Pseudoinverse rule [1,6] used for training single-layer networks.

One of the present authors has recently proposed another global learning rule, called the Monte Carlo adaptation algorithm (shorten as MCA algorithm hereafter) [7]. The basic idea is to make an adaptation to a randomly chosen synaptic weight, and accept the adaptation if it improves the network performance globally. A realization of the MCA algorithm had been used to train single-layer feedback neural networks with binary-state synaptic weights [7,8].

The purpose of this Letter is to present a general version of the MCA algorithm which is applicable to train multilayer neural networks with either continuous or discrete synaptic states, and with either differentiable or nondifferentiable neural transfer functions. Based on the observation that the network performance is determined by the local fields of neurons induced by the input of the samples (shorten as LFNIIS), our algorithm is focused on controlling the distributions of LFNIIS by continuously adapting the synaptic weights. Two steps are applied to perform the control. The first one is to determine the target distribution of the LFNIIS, define the states of synaptic weights, and chose the transfer function of neurons for each layer respectively. The second one is to randomly select a synaptic weight, and randomly adapt it to a new state, then make a decision whether or not to accept this adaptation by a criterion. This step is repeated till the distributions overlap with the target ones. The criterion for acceptable adaptations is crucial for the algorithm. In principle, we accept an adaptation if the distributions of LFNIIS induced by it does not diverge away from the target distributions statistically. This guarantees the distributions of LFNIIS evolving towards the targets in a one-way manner.

As a realization example of the above framework, we train a two-layer neural network to separate a set of linearly inseparable samples into two categories. In order to demonstrate the network not only overcomes the limitations of BP networks but also improves the network performance, we emphasize its powerful generalization capacity over a two-layer BP network. The generalization capacity is essential for a neural network. This is because the sample set is
where \( t \) inputting a vector which has a set of elements, denoted by \( \{ v_h \} \), network one obtains the local field, fields of the neurons in the hidden layer induced by this input should be \( h \) binary vector \( M \) that can be linearly separable is \( \text{hidden layer.} \)

represents the number of neurons in the \( l \) layer and \( \sigma \) is its transfer function. In the equation, \( N^{(l)} \) represents the number of neurons in the \( l \) layer with \( N^{(0)} \equiv N \).

A two-layer neural network has a hidden layer and a output layer. When the \( \mu \)th sample \( \xi^\mu \) is inputted into the network one obtains the local field, \( h^{(1)}_{i\mu} = \sum_{j=1}^{N^{(1)}} J^{(1)}_{ij} v_j \), and the output, \( v_{i\mu}^{(1)} = \sigma^{(1)}(h^{(1)}_{i\mu}) \), of the \( i \)th neuron in the hidden layer.

For the output layer, because we want the network to separate the samples into only two categories, one neuron in this layer is enough. In this case, the weight matrix will be a \( 1 \times N^{(1)} \) matrix, whose elements will be denoted by \( J^{(2)}_{ij} \). Here \( N^{(1)} \) is the number of neurons in the hidden layer. Inputting the vector \( v_{i\mu}^{(1)} \) to the output layer one obtains the local field, \( \tilde{h}^{(2)}_{i\mu} = \sum_{j=1}^{N^{(1)}} J^{(2)}_{ij} v_j^{(1)} \), and the output, \( \tilde{v}_{i\mu}^{(2)} = \sigma^{(2)}(\tilde{h}_{i\mu}^{(2)}) \), of the neuron.

Let \( \Sigma_1 \) and \( \Sigma_2 \) represent the two categories of samples. Our goal is to establish the connections, \( v_{i\mu}^{(2)} = 1 \) if \( \xi^\mu \in \Sigma_1 \) and \( v_{i\mu}^{(2)} = -1 \) if \( \xi^\mu \in \Sigma_2 \), by the proper solution of \( J^{(l)} \) and \( \sigma^{(l)} \). To fulfil this goal, the transfer function of the neuron in the output layer must be the step function: \( \sigma^{(2)}(x) = 1 \) for \( x \geq 0 \) and \( \sigma^{(2)}(x) = -1 \) for \( x < 0 \).

The establishment of the connections implies the satisfaction of the condition \( t_h^{(2)} \geq 0 \) in terms of the local fields, where \( t_h = 1 \) for \( \xi^\mu \in \Sigma_1 \) and \( t_h = -1 \) for \( \xi^\mu \in \Sigma_2 \). However, this is not enough for the generalization. When inputting a vector which has a set of elements, denoted by \( \{ k \} \), different from, say, the \( \mu \)th sample, then the local fields of the neurons in the hidden layer induced by this input should be \( \tilde{h}^{(1)}_{i\mu} = h^{(1)}_{i\mu} - 2 \sum_{j=1}^{N^{(1)}} J^{(1)}_{ij} \xi_j^\mu \), where the sum is over the set of \( \{ k \} \). This in turn results in a set of elements, denoted by \( \{ k' \} \), different from \( v_{i\mu}^{(1)} \) and leads to \( \tilde{h}^{(2)}_{i\mu} = h^{(2)}_{i\mu} - 2 \sum_{j=1}^{N^{(1)}} J^{(1)}_{ij} v_j^{(1)} \) for the neuron in the output layer, where the sum is over \( \{ k' \} \). The generalization capacity is thus determined by the capability of conserving the sign of \( h^{(1)}_{i\mu} \) and \( h^{(2)}_{i\mu} \) under as many mutations as possible of the sample \( \xi^\mu \), which requires the absolute values of not only \( h^{(2)}_{i\mu} \) but also \( h^{(1)}_{i\mu} \) as big as possible.

Thus, to gain better generalization capacity we should expect the distribution of \( h^{(2)}_{i\mu} \) satisfy the condition \( t_h^{(2)} \geq c \), where \( c \) is a positive parameter. For the hidden layer, there is no restriction on the sign of a specific \( h^{(1)}_{i\mu} \), we thus define \( d_i = \sum_{\mu=1}^{M} |h^{(1)}_{i\mu}| \) to roughly measure the mean absolute value of the local fields. To gain better generalization capacity we expect \( d_i \) to be as large as possible.

We apply the following procedure to train the network to find a set of solution of synaptic weights that guarantees the desired distributions of \( h^{(1)}_{i\mu} \) and \( h^{(2)}_{i\mu} \) be satisfied.

1. Initialize \( J^{(l)}_{ij} \) with \( J^{(l)}_{ij} \in \{ \theta_k^{(l)}, k = 1, ..., p \} \) randomly with equal probability; calculate \( h^{(1)}_{i\mu}, v^{(1)}_{i\mu}, h^{(2)}_{i\mu} \) and \( d_i \). Here \( \theta_k^{(l)} \) is a state of \( J^{(l)}_{ij} \).

2. Randomly select a \( J^{(l)}_{ij} \) and randomly adapt it to a new state \( \theta_k^{(l)} \); if \( l = 1 \) calculate

\[
\tilde{h}^{(1)}_{i\mu} = h^{(1)}_{i\mu} + (\theta_k^{(1)} - \theta_k^{(1)}) \xi_j^\mu, \\
\tilde{v}^{(1)}_{i\mu} = \sigma^{(1)}(\tilde{h}^{(1)}_{i\mu}),
\]
Then calculate\[\tilde{h}_{\mu}^{(2)} = \sum_{q=1}^{N^{(1)}} f_{ij}^{(2)} v_{iq}^{(1)},\]
and the sum is just over those index set \(\{\mu\}\) of \(\mu\) satisfying \(t_{\mu}h_{\mu}^{(2)} < c\) or \(t_{\mu}\tilde{h}_{\mu}^{(2)} < c\).

If \(\tilde{d}_i \geq d_i\) and \(n \geq 0\), renew the parameters, i.e., \(h_{ip}^{(1)} \leftarrow \tilde{h}_{ip}^{(1)}, v_{ip}^{(1)} \leftarrow \tilde{v}_{ip}^{(1)},\) etc., otherwise remain the old ones; return to step (2) till the condition \(t_{\mu}h_{\mu}^{(2)} \geq c\) is achieved and \(d_i\) can not be further enlarged.

With a set of parameters \(N = 1000, N^{(1)} = 1000, M = 2400, c = 30\), and applying the binary weights \(J_{ij}^{(1)} \in \{+1, -1\}\) while adopting the step transfer function for each neuron, we tested the above training procedure by separating the samples into two sets with equal samples. Without loss of the generality, we suppose \(\xi_{\mu}^{\mu} \in \Sigma_1\) for \(\mu = 1, ..., M/2\) and \(\xi_{\mu}^{\mu} \in \Sigma_2\) for \(\mu = M/2 + 1, ..., M\). Note that the samples are linearly inseparable since \(M > 2N\).

In Fig. 1(a) and 1(b) the up-triangles show the distributions of \(h_{ip}^{(1)}\) and \(h_{ip}^{(2)}\) respectively. It can be seen that \(h_{ip}^{(2)}\) distributes in the region of \(t_{\mu}h_{\mu}^{(2)} \geq 30\) correctly, and the distribution of \(h_{ip}^{(1)}\) shows a two-peak structure.

The two-peak structure is a consequence of controlling the distribution of \(h_{ip}^{(1)}\) by restricting \(d_i \geq d_i\) for acceptable adaptations. If merely employ \(n \geq 0\) as the criterion for acceptable adaptations, the distribution of \(h_{ip}^{(2)}\) can fulfil the condition \(t_{\mu}h_{\mu}^{(2)} \geq 30\) easily. However, the distribution of \(h_{ip}^{(1)}\) will be out of control. The open stars in Fig. 1(a) and 1(b) show the distributions of \(h_{ip}^{(1)}\) and \(h_{ip}^{(2)}\) respectively. It can be seen that \(h_{ip}^{(1)}\) distributes around the origin with a single-peak structure, while the distribution of \(h_{ip}^{(2)}\) is similar to that obtained by using \(n \geq 0\) and \(d_i \geq d_i\) as the criterion.

For the generalization, the distribution of \(h_{ip}^{(1)}\) with the two-peak structure is obviously preferable than that with the single-peak structure, since the amount of elements of \(h_{ip}^{(1)}\) with small absolute values in the former case is much less than that in the latter case. Figure 2 confirms this prediction. In the figure, the triangles and stars show the generalization capacity of the networks obtained with the criterion \(d_i \geq d_i\) and \(n \geq 0\), and with merely the criterion \(n \geq 0\), respectively. The horizontal axis is the mean percentage of the difference between an input vector and one of the samples. The vertical axis is the rate of correct classification. It is clear that the former network has much higher generalization capacity than the later one. Note that an input vector with no correlation with any sample has equal probability to be classified into either category, a rate of 0.5 therefore indicates the total loss of the generalization capacity.

By adopting the mean square error \(< (h_{ip}^{(2)} - c)^2 >\) as the performance index and the analog function \(\sigma^{(1)}(x) = tanh(x)\) as the transfer function for each neuron in the hidden layer, one can obtain a two-layer network capable of categorizing the same set of samples using the BP algorithm. In order to make comparison with our network, we apply \(c = 34\) and stop the learning procedure after the condition \(t_{\mu}h_{\mu}^{(2)} \geq 30\) is satisfied for all samples. The weights are normalized to satisfy \(< J_{ij}^{(1)} > = 1\). The dot-lines in Fig. 1 show the distributions of the LFNIIS for the BP network. It can be found that \(h_{ip}^{(2)}\) distributes around \(\pm c\) as two Guassian-like peaks, and \(h_{ip}^{(1)}\) distributes around the origin. Clearly, the distribution of the LFNIIS for the hidden layer is out of the control of the algorithm since \(h_{ip}^{(1)}\)
is not included in the performance index, and the two peaks in the distribution of $h_{ij}^{(2)}$ is induced by the operation of minimizing the mean square error. The minimization operation drives the local fields not only with smaller value but also with larger value of $t_{ij} h_{ij}^{(2)}$ concentrated towards $c$ synchronously, while the larger values are favorable for the generalization capacity as explained earlier. Thus, the generalization capacity of the BP network would be even worse than that of our network obtained with merely the criterion $n \geq 0$. The rate of correct generalization represented by the dots in Fig. 2 confirms this prediction.

Our procedure can be directly extended to train neural networks with synaptic weights having more discrete states. It can be found easily that when the states are extended to infinite, e.g., $J_{ij}^{(1)} \in \{\pm 1, \pm 3, \pm 5, \ldots \}$, the weights indeed become continuous (after been normalized). We have observed that the network performance can be further improved by increasing the discrete states. To show this, we made, between the networks with $J_{ij}^{(1)} \in \{\pm 1\}$ and the networks with $J_{ij}^{(1)} \in \{\pm 1, \pm 3\}$, a comparison of the maximum capacity of separating no-correlation samples into two sets with equal members. The weights in the output layer are fixed at $J_{ij}^{(2)} \in \{\pm 1\}$ for both networks. The results are shown in Fig.3, where $M/N$ is the normalized maximum amount of the samples that can be separated into two sets correctly within 0.01/NN times of repeat of the steps (2)-(3), and $N^{(1)}/N$ is the normalized number of neurons in the hidden layer. The up- and down-triangles represent the results for networks with $J_{ij}^{(1)} \in \{\pm 1\}$ and with $J_{ij}^{(1)} \in \{\pm 1, \pm 3\}$ respectively. In the calculation we fix $N = 500$. One can see from the figure that the maximum capacity increases as the increase of the neurons in the hidden layer, and increases with the increase of the discrete states of weights.

In summary, unlike the BP algorithm, the improved MCA algorithm puts no restriction to the neural transfer function and is applicable to train neural networks with either discrete or continuous synaptic weights. Another key difference is that we implement the desired network performance by controlling the distributions of the LFNIS, while the BP algorithm approaches this goal by minimizing the performance index defined constantly as the mean square error. It is obvious that one has a much wider freedom to improve the network performance by controlling the distributions of the LFNIS. This is because one has freedom not only to control the distribution for the output layer but also to control the distributions for the hidden layers. The good generalization capacity of the two-layer network trained with the criterion $d_i \geq d$ and $n \geq 0$ is just benefited from the control of the distribution of the LFNIS for the hidden layer.

The application of the algorithm described in this Letter to the problem of separating a set of samples into several categories is straightforward by involving more neurons in the output layer. The algorithm is directly applicable to train single-layer networks, and can be extended straightforwardly to train networks with three or more layers.

We want to emphasize that the MCA algorithm has capability for practical applications. For example, it takes about one hour of evolution time for a personal computer to train the network satisfy the condition $t_{ij} h_{ij}^{(2)} \geq 30$ by applying the criterion $n \geq 0$. To fulfil the same condition using the BP algorithm with optimal learning rate it takes about 6 computer hours.

It is necessary to point out that the training procedure is sensitive to technical details. For example, if one replaces the criterion $n \geq 0$ simply with $n > 0$ in the related training procedures above, it may need double the time to approach the same goals. On the other hand, certain treatments, such as adjusting the constant $c$ gradually to its target value, can dramatically decrease the training time. In addition, introducing temperature to the criterion for acceptable adaptations can affect the efficiency of training process in a complex way. These facts imply that there is a big possibility to further improve the training procedure.

Finally we briefly report an interesting phenomenon which may share lights on the role of different layers in a network. We have performed the MCA algorithm in two ways. One is to fix the weights in the output layer by some random realizations and merely adjust the weights in the hidden layer. The another is to adjust the weights in both layers. It was found that both ways can achieve the same goal of classification, but the training time used in the first way was dramatically less than that used in the second way. This implies that the role of the output layer is merely to span out the space. Each specific realization of weights for the output layer has a set of optimal realizations of the weights for the hidden layer, and every realization leads to the same target distributions of $h_{ij}^{(1)}$ and $h_{ij}^{(2)}$.

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FIGURE CAPTIONS

Fig.1 The distributions of LFNIS of (a) $h_{ij}^{(1)}$ and (b) $h_{ij}^{(2)}$.
Fig.2. The generalization capacity of the networks.
Fig.3. The maximum capacity of classification as functions of the neuron number in the hidden layer for $J_{ij}^{(1)} \in \{\pm 1\}$ and for $J_{ij}^{(1)} \in \{\pm 3, \pm 1\}$.
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